

THE ABSORPTION SPECTRUM OF H₂S BETWEEN 21S0 AND 4260 cm⁻¹:

**Analysis of the positions and Intensities in
the first [2v₂, VI and v₃] and Second [3v₂, v₁+v₂ and v₂+v₃] Triad Regions**

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Abstract

The two triad systems of hydrogen sulfide [2v₂, VI and v₃ near 4 μm and 3v₂, vi +v₂ and v₂+v₃ near 2.7 μm] were analyzed using fourteen spectra recorded at **0.0056** and 0.011 cm⁻¹ resolution with the McMath Fourier transform spectrometer located at Kitt Peak National Observatory. Experimental upper state levels of H₂³²S, H₂³⁴S and H₂³³S were obtained from assigned positions (as high as J = 20 and K_a = 15 for the main isotope). These were fitted to the A-reduced Watson Hamiltonian to determine precise sets of rotational constants through J¹⁰ and up to nine Fermi and Coriolis coupling parameters. Intensities of the two H₂³²S triads were modeled with rms values of 2.5%, using the transformed transition moment expansion with 19 terms for 568 intensities of the first triad and 11 terms for the 526 intensities of the second triad. The second derivatives of the dipole moment with respect to normal coordinates were estimated to be in Debye : ²²μ_x = -0.004873 (90); ¹²μ_x = 0.01372 (30); ²³μ_z = 0.01578 (30). This confirmed that for hydrogen sulfide some of the second derivatives are larger than the first derivatives. The calculated line intensities were summed yielding integrated band strengths in cm⁻²/atm at 296 K of : 0.3315 for 2v₂, 0.4522 for VI and 0.1201 for v₃, 0.0303 for 3v₂, 1.820 for v₁+v₂ and 2.869 for v₂+v₃. In addition, the hot band transitions were identified in both regions. Finally, a composite database of hydrogen sulfide line parameters was predicted for the 5 to 2.5 μm region.

I. Introduction

Detailed knowledge of hydrogen sulfide absorption spectra is important for terrestrial remote sensing applications and investigations of atmospheric chemistry in Venus and other planets. In the last dozen years, numerous studies of H₂S absorption at high resolution have been reported. As a result, the combined analyses of Flaud et al. [1], Yamada and Klee [2], Saleck et al. [3], Camy-Peyret et al. [4] and Belov et al. [5] have provided good ground state parameters for H₂³²S and its isotopes (H₂³³S, H₂³⁴S and H₂³⁶S and HDS). Likewise, the positions and intensities of its fundamentals and one overtone band up to 3000 cm⁻¹ are fairly well-characterized through the work of Strew [6], Lane et al. [7], and Ulenikov et al. [8] for v₂, and Lechuga-Fossat et al. [9] for

v_1 , v_3 and $2v_2$ [the first triad]. Some positions of the higher states of H₂S are also analyzed: Ulenikov et al. [10] for v_1+v_2 , v_2+v_3 and $3v_2$ at 2.7 μm; Zotov et al. [11] at 2 μm; Lechuga-Fossat et al. [12] at 1.6 μm (which also includes intensities); Flaud et al. [13] and Child et al. [14] at 0.82 μm, Bykov et al. [15] from 0.9 to 5 μm, and Vaittinen et al. [16] at 0.8 μm. Portions of the HDS spectrum are assigned as well [see 17,18 and the references therein].

The present paper is a continuation of our effort to analyze high resolution H₂S absorption spectra from 2000 to 11500 cm⁻¹ using the Fourier transform spectrometer at Kitt Peak. Previously, the observed band centers for 30 states were assigned and fitted in a vibrational analysis, and local mode behavior was demonstrated in four bands near 1 μm [15]. The resulting vibrational calculation proved satisfactory enough to predict [within 0.4 cm⁻¹] the $3v_1+2v_3$ and $2v_1+3v_3$ band centers observed later near 12149.458 cm⁻¹ by Flaud et al. [13], and to predict within 0.07 cm⁻¹ the highly excited $4v_1+v_3$ and v_1+4v_3 vibrational bands investigated at 12524.637 and 12525.214 cm⁻¹ in [16]. In the present study, we report the measurements and analyses of the positions and intensities of the first and second triads between 2200 and 4100 cm⁻¹. This spectral interval contains two parallel bands, v_3 and v_2+v_3 , at 2628 and 3789 cm⁻¹, respectively and four perpendicular bands, $2v_2$, v_1 , $3v_2$, v_1+v_2 , at 2353, 2614, 3514 and 3779 cm⁻¹, respectively.

II. Theoretical considerations

From symmetry considerations, one would expect that the III' representation of the A- or S-reduced Watson Hamiltonian could be used to model the bands of a near-oblate C_{2v} asymmetric rotor like H₂S. However, as demonstrated by Strew [6] and reiterated recently by Yamada and Klee [2], this choice results in much slower convergence and poorer fits to experimental data because of the magnitude of the S₁₁ term. As a result, many investigators have selected the A-I' scheme to model the ground state and vibrational bands, and we have adopted their approach for our studies. This choice then permits direct comparison of our fitted constants with those in the literature. We have also elected to use the older ground state constants of Flaud et al. [1] rather than the results of the recent studies [2,5] because the older study fitted data up to J = 22 and K_a = 15 to an rms of 0.00035 cm⁻¹. While the new rotational parameters and the S-reduced and the Pade form of the A-

reduced Hamiltonians are better for reproducing the highly accurate millimeterwave and sub-millimeterwave transitions for $J \leq 15$, they do not provide the necessary accuracy for the higher J levels in our data (see Table IV of Belov et al. [5]).

For HzO-type molecules, it is well known that Coriolis and Fermi-type resonance couplings must be taken into account to calculate precisely the rotation-vibration energy levels of triad states. As a consequence, the effective rotational Hamiltonian has the form:

$$H = \sum_{V,V'} |V\rangle H_{VV'} \langle V'| \quad (1)$$

where, following Lechuga-Fossat et al. [9], diagonal operators H_{VV} are taken as Watson-type A-reduced Hamiltonian :

$$\begin{aligned} H_{VV} = & E^V + \left[A^V - \frac{1}{2} (B^V + C^V) J_z^2 + \frac{1}{2} (B^V + C^V) J^2 - \Delta_K^V J_z^4 \right. \\ & - \Delta_{JK}^V J_z^2 J^2 - \Delta_J^V J^4 + H_K^V J_z^6 + H_{KJ}^V J_z^4 J^2 + H_{JK}^V J_z^2 J^4 \\ & + H_J^V J^6 + L_K^V J_z^6 + L_{KKJ}^V J_z^6 J^2 + L_{KJ}^V J_z^4 J^4 + L_{KJJ}^V J_z^2 J^6 \\ & + L_J^V J^8 + P_K^V J_z^{10} + P_{KKJ}^V J_z^8 J^2 + P_{KJJ}^V J_z^6 J^4 + \dots \quad (2) \\ & + \frac{1}{2} (B^V - C^V) J_{xy}^2 - \delta_K^V \{ J_z^2, J_{xy}^2 \} - 2\delta_J^V J_{xy}^2 J^2 + h_K^V \{ J_z^4, J_{xy}^2 \} \\ & + h_{KJ}^V \{ J_z^2, J_{xy}^2 \} J^2 + 2h_J^V J_{xy}^2 J^4 + l_K^V \{ J_z^6, J_{xy}^2 \} + l_{KJ}^V \{ J_z^4, J_{xy}^2 \} J^2 \\ & + l_{JK}^V \{ J_z^2, J_{xy}^2 \} J^4 + 2l_J^V J_{xy}^2 J^6 + p_K^V \{ J_z^8, J_{xy}^2 \} + p_{KKJ}^V \{ J_z^6, J_{xy}^2 \} J^2 + \dots \end{aligned}$$

and non-diagonal operators $H_{VV'}$ for Coriolis interaction have the form:

$$\begin{aligned} H_{VV'} = & C_y^{VV'} iJ_y + C_x^{VV'} \{ J_z, J_x \} + C_{yz}^{VV'} iJ_y J^2 \\ & + C_{xzK}^{VV'} \{ J_z^3, J_x \} + C_{yK}^{VV'} iJ_y, J_z^3 + C_{xzJ}^{VV'} \{ J_z, J_x \} J^2 \quad (3) \end{aligned}$$

and for Fermi-type resonances :

$$H_{VV'} = F_K^{VV'} J_z^2 + F_J^{VV'} J^2 + F_{xyK}^{VV'} J_z^2, J_w^2 \quad (4)$$

where $J_{xy}^2 = J_x^2 - J_y^2$ and $\{A, B\} = AB + BA$.

The matrix elements of the Hamiltonian are calculated using the basis functions $|V\rangle|JKT\rangle$, where $|JKT\rangle$ are Wang's symmetry adapted rotational wavefunctions. Diagonalization of this matrix gives the energy levels values and the corresponding wavefunctions, which are a linear combination of the basis functions with the coefficients C_{JK}^V :

$$|V_1 V_2 V_3 JK_A K_C \Gamma\rangle = \sum_{VA} C_{JK}^V |V\rangle|JKT\rangle \quad (5)$$

Here and in Eqs. (1) - (4), $|V\rangle, |V'\rangle$, stand for $V_1 V_2 V_3\rangle, |V\rangle = 001, 100, 020$ - for the 1st triad, $|V\rangle = |011\rangle, |110\rangle, |030\rangle$ - for the 2nd triad.

To estimate resonance couplings between different states, the mixing coefficients are used

$$\%_o(V) = \sum_K (C_{JK}^V)^2 \quad (6)$$

Our results are expected to follow those of Lechuga-Fossat et al. since the 2nd triad upper states [(030), (110), and (011)] are basically the states of the first triad [(020), (100), and (001)] with one additional quantum of V_2 activated. Thus the principal interactions are Coriolis terms linking (011) with (110) and (030) and the Fermi terms between the (110) and (030) states.

The calculation of asymmetric rotor line intensities is well-established [19-22] and closely follows that of Lechuga-Fossat [9]. The intensity of a transition between an initial $|i\rangle$ and final state $|f\rangle$ in units of $\text{cm}^{-2}/\text{atm}^{-1}$ at a given temperature T is given by

$$I_{ij} \left(\text{cm}^{-2} / \text{atm} \right) = \frac{8\pi^3}{3hc} L \cdot a_i \frac{T_0}{T} \frac{g_i}{Z(T)} v_{if} \left[1 - \exp \left(-\frac{hc v_{if}}{kT} \right) \right] \times \exp \left(\frac{-E_i}{kT} \right) \langle i | \mu' | f \rangle^2 \quad (7)$$

In these expressions, c is the velocity of light; h is the Planck constant; k is the Boltzmann constant; L is Loschmidt's number = 2.686754×10^{19} ; $Z(T)$ is the partition function (where $Z(T) = 505.6$, 506.3 and 506.9 for H_2^{32}S , H_2^{33}S , H_2^{34}S , respectively at 296 K); g_i is the degeneracy due to the nuclear spin of the lower state (3 for K_a - KC odd and 1 for K_a - KC even); v_{if} is the transition frequency; T_0 is the standard temperature 273.15 K; a_i is the isotopic abundance (0.950, 0.0422 and 0.0078 for ^{32}S , ^{34}S and ^{33}S respectively); and E_i is the lower state energy. The transformed dipole moment operator μ'_z has the form:

$$\mu'_z = \sum_v |0\rangle \langle v | \mu'_z \langle V | = \sum_v |0\rangle \left| \sum_{j=1}^8 {}^v \mu'_j {}^v A_j \right| \langle V | \quad (8)$$

In (7)-(8), $|i\rangle = \sum C_{JK}^{(000)} |000\rangle |JKT\rangle$, $|f\rangle = \sum_{VK} C_{JK}^V |V\rangle |JKT\rangle$, and $|V\rangle$ are the 1st or 2nd triad vibrational functions, ${}^v \mu'_j$ are parameters and "A_j" are the combinations of angular momentum operators and direction cosines given for asymmetric rotors by Camy-Peyret and Flaud [19-22] for j up to 8. In this expansion, $j = 1$ is the effective dipole moment associated with the vibrational mode. The higher order terms account for rovibrational interactions in a manner similar to the much simpler Herman-Wallis factors for linear molecules. Unlike the very simple expression for linear molecules (which depend on J or m), the matrix elements of these terms affect the intensities as a complicated function of J, AJ, K and AK. However, as shown in Table XIV of [22], the observed transition moment coefficients for the H_2S fundamentals are very well reproduced by the theoretical expressions relating the expansion coefficients to basic molecular constants of H_2S .

The term total band strength is defined to mean the sum of all individual transition intensities of a band up to a given J_{\max} . This is often computed using a minimum intensity criterion that excludes very weak lines from the summation.

$$S_r = \sum_{I_{ij} \geq I_{\text{min}}} I_{ij} \quad (9)$$

111. Experimental details and data reduction.

Laboratory spectra of H₂S were recorded at 0.0056 and 0.011 cm⁻¹ resolution with the McMath Fourier transform spectrometer located at Kitt Peak National Observatory/ National Solar Observatory. The experimental conditions are summarized in **Table 1**, and an observed spectrum is shown in **Figure 1**. The 0.011 cm⁻¹ resolution data were obtained using CaF₂ beamsplitters and InSb detectors while the two spectra at 0.0056 cm⁻¹ resolution were recorded with KCl beamsplitters and As-Si detectors. Four different stainless steel absorption cells were used to achieve optical paths from 0.25 to 433 m, and the H₂S pressures were varied from 1.49 to 90 torr at room temperatures between 289 and 297 K. With globar sources, it was possible to produce signal to noise ratios of 500:1 or better by integrating each spectrum 70 to 80 minutes. Gas pressures were monitored continuously during the scans using Baratron capacitance gauges, and temperatures were measured by thermocouples in contact with the exterior of the absorption cells. For some scans, a second absorption cell containing CO was placed in series with the H₂S cell to establish the frequency calibration using the 2-0 and 1-0 positions reported respectively by Pollock et al. [23] and Maki and Wells [24]. Because the FTS chamber was evacuated to only 0.015 torr, residual absorption of CO₂ and H₂O appeared in all the spectra. In fact, for the 2nd triad, this interference was quite severe, and in **Fig. 1**, all the strong lines near 3700 cm⁻¹ belong to water rather than H₂S. The residual water absorption at 3800 cm⁻¹ [25] and 5300 cm⁻¹ [26] were also used as calibration standards (the H₂O transitions between 5250 and 5350 cm⁻¹ were referenced against the 2-0 band Ofco [23]).

The line centers were determined either by doing first and second derivatives of the apodized spectra or by least-square fitting of the Voigt contour with the unanodized data [as described in Brown et al. (27)]; the second method produced the measured intensities. **Figure 2**

gives an example of the measurement technique applied (to the features at 3717.8 cm^{-1}). The bottom panels show the observed and synthetic spectra overlaid after the adjustment the positions, intensities and line widths; the top panel shows the residual differences in percent. The last column of **Table 1** indicates which runs were used for line positions and the calibration standards. Most of the positions came from lower pressures spectra; the other two scans were used in the wings of the region. Intensities, while obtained from all 14 scans listed in **Table 1**, were generally averaged values of 2 to 9 spectra. At the end of the study, additional data were needed for intensities of transitions greater than $0.001\text{ cm}^{-2}/\text{atm}$, and self-broadening coefficients (which are being reported separately [28]) were obtained as part of the intensity data reduction. The spectral data were not of sufficiently enough high pressure, however, to determine accurate self-broadened pressure shifts for most lines. A comparison of line centers from the 1.49 Torr and 90 Torr runs revealed differences mostly in the range of 0.0001 to 0.001 cm^{-1} with 40% of the shifts being positive and 60% negative. A few differences were as high as 0.003 cm^{-1} . These comparisons indicated that most of the observed line centers are pressure-shifted by 0.0003 cm^{-1} or less in the four spectra used for determining line positions. The precision and accuracies of the observed positions were also estimated by comparing with known CO standards and doing H₂S ground state [1] combination differences. With the wavenumber (cm⁻¹) calibration, the rms between the measured and standards CO positions was 0.00005 cm^{-1} after the observed positions had been multiplied by a constant. However, due to the overlap of H₂S transitions with each other and residual H₂O features, the accuracies were degraded. The combination differences indicated that the precisions range from 0.00020 cm^{-1} for well-isolated strong transitions to 0.003 cm^{-1} for unresolved blends. All things considered, the absolute accuracy of the positions of isolated features is thought to be 0.0003 cm^{-1} or better.

The precision of the intensities were initially judged by comparing the internal consistency of the individual measurements. The rms agreement between values obtained from different spectra was computed, and measurements with rms values worse than 8% were discarded. Comparison of intensities obtained with different detectors in the 2200 to 2600 cm^{-1} interval revealed no systematic differences. However, it was noticed that the runs involving the 16.4 m paths in **Table 1** gave intensities that were 8% lower than the data obtained with shorter cells and two different detectors.

To improve precision, the longer path data were rescaled to match. It is thought that the resulting precision of isolated lines are in the range of 2 - 3%, but the absolute accuracy of the band strengths is 4% or better.

II. Spectrum assignment

The first triad was completely assigned by the earlier work [9] (up to $J = 20$ and $K_a = 14$ for the main isotope) so that the present data were easily interpreted. With the second triad, we learned of the Ulenikov et al. [10] study only after we began writing the present paper, and thus we made our identifications independent] γ between 3200 and 4100 cm⁻¹. For this process, transitions were identified using approximate predictions and the method of combination differences. The ground state (000) levels were calculated with the rotational constants from [1]. Initially, the rotational constants for the (O 11) and (11 O) states of $H_2^{32}S$ were taken from [29] while those of (030) were estimated from the parameters of the (O 10) and (020) states. The predictions of the triad were then further refined by fitting observed upper state levels and preliminary line intensities based on one spectrum. With the better prediction, assignments at higher J values were readily obtained. By repeating this procedure many times, we finally were able to assign with confidence even the weak lines which have no combination pairs.

The same procedure was followed to assign the $H_2^{33}S$ and $H_2^{34}S$ lines. The initial estimations for rotational and centrifugal distortion constants were made using isotopic rules:

$$A_{iso}^{V_1 V_2 V_3} = A_{main}^{V_1 V_2 V_3} \frac{A_{iso}^{000}}{A_{main}^{000}} \quad (10)$$

where A - is a rotational or centrifugal distortion constant. For the ^{34}S isotope, the band centers were calculated in the manner of [15], and the ^{33}S band centers were estimated to be the average of the other two isotopes. For the weaker transitions, the assignment process relied generally on the predictions since the combination differences were absent due to the overlap of stronger lines. To check for coincidences with hot band lines, the transitions of $4v_2-v_2$, $2v_2+v_3-v_2$ and $v_1+2v_2-v_2$ were predicted using the experimental rotational energy levels and rotational parameters for (040), (120)

and (02 1) [30] while the hot bands in the first triad regions were predicted using our upper state constants for (030), (11 O) and (O 11) and the (O 10) constants of [8] for the lower state.

The process of finding the correct combination differences in the experimental spectrum was performed with the aid of the special computer program developed by A. Scherbakov [31]. This software used pattern recognition algorithms and functioned in many modes: from searching the ground state combination differences in a wide range when the upper states parameters were approximate, to finding single lines in the spectrum, which had the line centers and intensities close to calculated ones once the upper state parameters were known accurately.

V. Results and Discussion

The assigned positions belonging to the two triads were combined with calculated ground state energies [1] to produce experimental upper state levels, which were in turn fitted to the Watson Hamiltonian. The resulting wavefunctions were used to model experimental intensities and obtain the transition moment parameters. Different combinations of interaction terms were tried in both the energy and intensity fits as additional data were included. In both triads, the resonances of weak and strong bands had a marked effect on the intensities. It was possible to select a combination of resonance parameters to improve the energy levels fit, but at the expense of the intensities fit for the weaker bands. Since our goal was to create a good molecular database for H₂S, special efforts were made to maintain quality for the intensity fit even though the calculated positions were degraded a bit..

The results are given in **Tables 2-9** and the Appendices. In **Table 2**, an overview of the measurements and results is given by showing the band, isotope, numbers of upper state levels (on the left) or transition intensities (on the right), the maximum values of upper state J and K_a and the rms of the observed minus calculated values in cm⁻¹ for positions and % for intensities. **Tables 3-5** list the fitted rotational parameters of the triads for the three isotopes respectively. The fitted

parameters of the transformed transition moment operator are presented in **Table 6** while the experimental energy levels appear in Appendix I. **Table 7** shows wavefunction mixing examples within the second triad. In **Table 8**, the observed and predicted [32] transition moment derivatives with respect to the normal coordinates are compared for the main isotope. **Table 9** lists integrated intensities with the corresponding measurements in Appendices II and III. Surprisingly, the second triad combination bands were found to be several times stronger than the first triad fundamentals.

V. 1 First triad upper state levels

In this case, the prior [9] rotational and transition moment parameters permitted quick identification of transitions; from these observed positions, 723, 377 and 179 accurate energy levels for (001), (100) and (020) states of H_2^{32}S , H_2^{34}S and H_2^{33}S were derived. The experimental energy levels of the present and prior studies were rather similar; 149 of their energy levels were not seen in our spectrum (partly because they used higher optical densities), but we derived 211 new levels. The largest number of the new experimental energy levels was obtained for H_2^{33}S molecule. The two sets of experimental energy levels lists were generally consistent with each other to within $\pm 0.0015 \text{ cm}^{-1}$; the absolute average deviation varied from 0.0003 cm^{-1} for small values of rotational quantum numbers J to 0.0005 cm^{-1} for high J numbers. There is also small negative shift about 0.0005 cm^{-1} between the prior study and our (020) vibrational state energy levels that was especially noticeable for small J values; this was perhaps caused by the revision of accepted calibration standards [33]. Some energy levels in both lists differ up to 0.003 cm^{-1} due to different line choices in the combination difference or a difference in the observed line centers.

While the prior results [9] accounted for almost all our observed transitions, their parameters did not reproduce the experimental accuracies of our energy and intensity data; their observed-calculated deviation (RMS) was 0.0050 cm^{-1} and 10% respectively. For this reason, we decided to refit the first triad for all three isotopes. With the energy levels, we found that including additional “diagonal” and resonance parameters into the fitting yielded considerably better rms deviations (0.00041 cm^{-1} for the H_2^{32}S triad). For this, 79 “diagonal” and 7 resonance parameters were used in the fitting instead of the 55 “diagonal” and 3 resonance in Ref. 9. The ratio of our

observed levels to fitted parameters was **8.4**, compared to a ratio of 12.4 in Ref. 9. The fitted parameters are presented in **Table 3** together with 68% confidence intervals.

The correct interpretation of the resonance interactions between the triad levels was found to be very important in achieving the higher quality fit. The Coriolis-type resonances between (00 1) and (100) and (020) and (001) were discussed in Ref. 9; the first was very strong with resonance mixing of the wavefunctions up to 48%, and the second was much weaker with the largest resonance mixing being only 3.8%. In our re-analysis, we also found that the “weak” Fermi-type resonance interaction between (100) and (020) was required to reproduce the high accuracy data even though the mixing was generally small. Besides the usual Coriolis-type C_y, C_{xz} resonance parameters, the C_{yk} parameter (see Eq. 3) was varied. Using such additional Fermi and Coriolis-type resonance terms is not unusual, particularly for H_2S (see Refs. 10 and 13). In a recent theoretical paper of Starikov [34], the necessity of including such parameters in the resonance blocks was demonstrated for different types of the interacting states. It should be noted that the same quality fitting can result by varying different combinations of the rotational and resonance parameters. For example, nearly the same runs deviation for the first triad levels was obtained with C_y [(020),(001)] equal to zero, but the intensity fit was slightly poorer. In the end, the accurate intensity data (discussed later) guided our interpretation of the interaction scheme and our choice of which parameters to adjust.

The evaluation of experimental energy precision was also revisited. in the previous paper [9], the experimental uncertainties in the majority of energy levels were believed to be from 0.0008 to 0.003 cm⁻¹ for $J \geq 11$. However, we concluded that the real precision of the experimental energy levels in our (and their data) were much better. For our data, the average experimental uncertainty obtained from the combination differences (with two to four transitions) was equal to 0.00018 cm⁻¹ with 507 of our “good” $H_2^{32}S$ levels. The remaining 216 experimental energy levels in our list were derived from single lines, but we decided that the uncertainty of this subset levels was not much worse than for the first group since there was no significant difference between the observed - calculation deviations. In reality, a large number of our “single line” levels originally were based on combination differences in which one of the transitions was poorly measured; these levels were “cleaned” by choosing another line which reduced the observed -calculated deviation.

We therefore concluded that the rms of the fit up to $J = 20$ (0.0004 I cm^{-1}) is close to our experimental precision (0.0003 cm^{-1}).

Once the spectroscopic parameters for the first triad of the H_2^{32}S molecule were obtained, it was an easy task to fit the corresponding parameters of the same bands of H_2^{34}S and H_2^{33}S molecule. Since the number of experimental data for H_2^{33}S and H_2^{34}S molecules was less than for main isotope, it was not possible to vary some of the higher-order centrifugal distortion and resonance constants. For this reason, some resonance parameters were simply fixed to the retrieved H_2^{32}S values, but the higher centrifugal distortion constants were fixed to isotonically adjusted values computed with Eq.(10). It should be noted that the energy levels structure and resonance picture for the isotopic species are very similar to those of the main isotope. So we were able to reproduce large number of isotopic energy levels using significantly fewer varied parameters. Finally, the rms deviation of 0.00047 cm^{-1} was obtained for 377 energy levels and 36 fitted parameters of H_2^{34}S . For H_2^{33}S isotopic states, the rms deviation was 0.00062 cm^{-1} for 179 experimental energy levels with 23 varied parameters. The poorer rms deviations in this case reflected the poorer experimental accuracy of the measured positions for weak lines and the absence of combination differences for majority (148) of the levels. The spectroscopic parameters of the H_2^{34}S and H_2^{33}S species are presented in **Tables 4 and 5** together with 68% confidence intervals. The increased accuracy of our first triad analysis allowed us to locate 211 new experimental energy levels for all three isotopic species with generally higher J and K_a values. From the 149 missing in our list energy levels from Ref. 9, 109 coincide with our calculation within $\pm 0.0017 \text{ cm}^{-1}$, and only 14 assignments were not confirmed by our calculations.

V.2 First Triad Intensities

Intensity measurements for the first triad were initially done with a few spectra to check the consistency of the new data with the prior study [9]. However, it was found that the values calculated using the rotational, coupling constants and transition moment parameters permitted an observed - calculated intensity rms of only 10%. (Ultimately, nine of the spectra in **Table 1** were used to retrieve new intensities for 568 “clean” lines (151 for v_3 , 249 for v_1 and 168 for $2v_2$,

including doublet lines). Finally, 19 parameters of the transformed transition moment operator were obtained in a fit which reproduce the experimental intensities with the average rms error of 2.4%. The fitted intensity data are shown in Appendix 11. The transformed transition moment parameters are presented in **Table 6** together with 68% confidence intervals along with the prior parameters [9].

The two sets of parameters differ slightly because of differences in experimental data. Beginning around 2700 cm⁻¹, our experimental intensities are greater than Ref. [9] data by about 14%. At the same time, their calculated data are lower than the experimental ones throughout by 6 to 8% on average so that the deviations between their calculated and our observed data reach the average value of 18 % for frequencies larger than 2700 cm⁻¹. These differences are to be expected because of the way their intensities were obtained. Their data reduction for intensities relied on the method of equivalent widths rather than curve fitting. Due to computer memory limitations, their spectra were recorded in two segments (at 0.01 cm⁻¹ resolution with a Bomern FTS), and the 2700 to 2750 cm⁻¹ interval was the overlap region between two bandpasses. They used a total of three spectra to cover a pressure range that varied by a factor of 25. Thus, for most of the transitions, the measured intensities were based on just one spectrum rather than being an average of several spectra. In our own data, we saw the value of using multiple optical densities to obtain good results. We initially started with over 600 empirical intensities; some were measured from only two or three spectra while more were obtained with four to nine scans. In the process of discarding measurements by comparison with the calculated values, we found that 80% of the removed lines came from intensities based on two and three spectra, and only 1 line of the rejections were obtained with five scans. In the prior study [9], they correctly assessed the accuracy of their intensity data to be no better than 10%, and pushed their modeling accordingly. We judged our precision to be around 3% and varied the model to achieve a better quality fit.

V.3 Second triad upper state levels

For the second triad, our assignment procedure (done independently of Ref. 10) resulted in 750 accurate energy levels of (01 1), (110) and (030) vibrational states of ³²S isotopic species up to J

$= 20$ and $K_a \leq 15$. These levels were typically determined from two or more line centers with experimental uncertainties varied from 10^{-4} to 10^{-3} cm^{-1} , but for high values of quantum number J many levels were obtained from only one line center. For ^{34}S isotopic variant 444 experimental levels were found for all second triad members up to $J = 18$ and $K_a \leq 13$. For the ^{33}S isotope, 257 energy levels were derived mainly belonged to the combination bands up to $J = 16$ and $K_a \leq 10$. Only 12 energy levels were found to the (030) state. The experimental energy levels are presented in **Appendix L**. These were fitted with the average deviations of 0.00052 cm^{-1} for H_2^{32}S , 0.00039 cm^{-1} for H_2^{34}S and 0.00065 cm^{-1} for H_2^{33}S to obtain the Hamiltonian constants in **Tables 3 - 5**. For ^{32}S , the ratio of observed levels to fitted parameters was 8.

The vibrational state pairs [(01 1), (110)] and [(100), (001)] are so close together (with separations in the vibrational energies of 10 cm^{-1} and 14 cm^{-1} respectively) that the Coriolis coupling between them is very strong. In the second triad, the effect is apparent from $J=3$ to the maximum $J (=20)$ assigned, and there are many perturbations at every value of J . The examples of the most perturbed energy levels for different values of J are listed in **Table 7** together with the mixing coefficients in %. The calculated energy levels are marked by asterisks. For instance, [8 5 3] (01 1) and [8 6 3] (110) states are mixed almost equally so that the labeling of such states becomes somewhat arbitrary. In contrast, the energy level structure of (030) state is very different from that of the (01 1) and (11 O) states because of the large gap in vibrational energies (about 270 cm^{-1}) and because of the big difference in the bending v_2 quantum numbers. For this reason Fermi-resonance interaction between (11 O) and (030) affects our modeling only from $J = 11$ while the Coriolis resonance between (01 1) and (030) begins only at $J = 12$. The interaction with (030) state is not as pervasive as the Coriolis (01 1)-(110) resonance: it perturbs only separate levels for given value of J , but for some levels resonance mixing is very large. For instance, mixing between [149 5] (011) level and highly excited [14 12 3] (030) level is equal to 29%. From the mixing coefficients analyses it is also obvious that for (030) the Coriolis resonance is much stronger than the Fermi. For some cases it seems, that Fermi resonance between (11 O) and (030) states is indirect and manifests itself often through the strong link between (110) and (O 11) levels, when the latter are perturbed by (030) state. It is always of great interest when otherwise extremely weak lines become detectable as a result of borrowing intensity from other vibrational transitions via large cross terms in the wave

functions. In our case, two levels of (030), [12 9 3] and [14 12 3] give rise to observed transitions due to resonance intensity redistribution in our data. Such assignments give us very important information for evaluating of the high-order (030) constants and lead to a better prediction of higher quanta (030) levels.

At first, it was difficult to account for the resonance with bending state. The high J and K_a (030) levels that were involved in resonance gave rise to weak transitions that we could not observe. On the other hand, for the levels of (O 11) and (11 O) that were strongly perturbed by (030), the proper calculation finally required four new Coriolis and one Fermi-type resonance parameters (see formulas (3) and (4)) in addition to the conventional two Coriolis and four Fermi constants. As with the first triad, this interpretation was also in agreement with a recent theoretical investigation of Starikov [34], where it was shown that when highly excited bending states of the light nonrigid molecules are involved in resonance interactions, a new type of Hamiltonian reduction takes place for the resonance blocks, allowing for the existence of the additional resonance parameters. Some high order “diagonal” parameters of (030) state were also included into the fit for the same reason, as mentioned above, despite the lack of observed (030) levels at high J and K_a . Therefore, the values of these parameters are thought to be somewhat “effective”.

It should be stressed, that the manifestation of the (01 1)-(030) and (110)-(030) resonance for $J \geq 14$ levels became a critical point for our fitting. The RMS value increased from 0.00031 cm^{-1} for all $J \leq 13$ levels to 0.00037 cm^{-1} when the $J = 14$ levels were included. This is a consequence of the strong mixing (up to 35-40%) of several $J = 14$ (O 11) and (110) levels with highly excited ([14 12 3], [14,14 1] and [14 14 2]) of (030) levels. For the most part, contribution of the new resonance parameters began with $J = 14$. The complicated resonance interactions and increasing of the rotational excitation up to $J = 20$, together with the decreasing of the experimental accuracy for weak highly excited transitions involved into the fitting, finally yielded an overall rms of 0.00052 cm^{-1} .

Once the H_2^{32}S second triad energy spectrum was well understood and reproduced, the H_2^{33}S and H_2^{34}S energy levels were readily obtained and modeled. As in the first triad, some centrifugal and resonance constants were calculated using Eq. 10 or fixed to the main isotope

parameters. The correctness of the resonance parameters of the main isotope was confirmed by very good prediction of the $H_2^{33}S$ and $H_2^{34}S$ resonance scheme despite the fact that resonance interactions in the isotopes were slightly shifted. For instance, Fermi-type resonance between (110) and (030) states begins from $J=10$ and Coriolis [(011),(030)] resonance takes place from $J=13$ for both the ^{34}S and ^{33}S isotopes. The resonance interactions in the second triad of $H_2^{34}S$ seemed to be rather numerous and required 6 resonance constants in the fit. For $H_2^{33}S$, only the four largest coupling constant were refined.

The rotational and centrifugal distortion constants of the 2nd triad were very consistent with those of (010) [8] and (100),(001),(020). For example, for the combination bands, the rotational constants B and C are within 0.0001 cm^{-1} or better of the values obtained by adding the differences between v_2 and the ground state to the fitted parameters of (100) and (001). As expected, the excitation of each bending quanta leads to increasing values of A , Δ_k , H_k and other parameters from so-called J -sequence of the Hamiltonian. This increase is large for the higher order constants; in our case the value of L_k parameter of (110) is more than twice the L_k of (100). The values of δ_k for (011), (110), (100),(001) states are negative, but for (020),(030) this constant is positive. This fact is in agreement with other studies of excited vibrational states [10] and can be explained by a strong vibrational dependence of the δ_k parameter on the v_2 quantum number in water-like molecules. The centrifugal distortion parameters for both triads have the same signs, but for δ_k constants, and are very close to each other for vibrational states with the same v_2 quantum numbers.

The comparison of our first and second triad resonance constants is not as straightforward because the analyses required slightly different combinations of resonance parameters. For the [(011),(110)] interaction, both C_y and C_{xz} parameters are close to the corresponding [(001),(100)] constants. In contrast, the resonances between [(011),(030)] and [(110),(030)] are much stronger than the corresponding first triad [(001),(020) and (100),(020)] interactions, and the perturbations become much more pervasive within the higher J and K_a levels of the second triad. For example, the largest mixing between the (100) and (020) states is only 0.5%, and 3.8% between the (001) and (020) states. It was also found that the set of resonance parameters used for the first triad did not work as well for the 2nd triad [(011),(030)], [(110),(030)] interactions. In particular, C_y for the [(011),(030)] resonance seemed to be undeterminable, whereas it had a rather large value for

$[(00\ 1\),(020)]$ interaction. On the other hand, the well-known ambiguities associated with the selecting sets of resonance parameters is demonstrated by the fact that a very similar rms can be reached for the first triad energies using the set of resonance parameters chosen for the second triad. In the end, the intensity modeling was done in parallel with the fitting of the energy levels so that selected set of parameters could be less arbitrary.

Finally, we compared our second triad energy levels and fitted parameters with those of Ulenikov et al. [10]. In that study, they recorded fewer spectra in segments and at a factor of four lower optical density, but they used higher resolution (Doppler-1 imited at $0.008\ \text{cm}^{-1}$ compared to our $0.011\ \text{cm}^{-1}$). The objective of their study was the assignment of the spectrum and the modeling of the positions of three isotopes; they also identified two hot bands. For ^{32}S , ^{34}S , ^{33}S of the second triad, they obtained, respectively, 438, 207, 80 upper state levels up to $J = 18$ and $K_a = 10$. They used 80 fitted rotational and interaction parameters to reproduce 352 energy levels of H_2^{32}S to a reported rms of $0.00013\ \text{cm}^{-1}$; the ratio of observed data to fitted parameters was 4.4. Working independently, we confirmed most of their assignments with a few exceptions for $3\nu_2$ of H_2^{33}S . We also noticed some systematic differences in the our and their observed positions and energies. Their sample positions and energies levels were higher by 0.0003 to $0.0005\ \text{cm}^{-1}$. Their fitted bands centers of the combination bands were within $0.0001\ \text{cm}^{-1}$ of ours values, but their overtone was higher by $0.0008\ \text{cm}^{-1}$. Part of these differences are perhaps related to different choices of calibration standards; they used C_2H_2 [35] in one spectrum and transferred the calibration to their other two scans while we used CO [23]. However, there is no ready explanation for our differences in the (030) levels. Thus, while the rms of their fitted positions is better than ours, we do not confirm that their absolute accuracy is as good as the inherent precision of their positions. We also found that their fitted constants did not extrapolate for the $J \geq 14$ levels. We traced both large (up to $0.1\ \text{cm}^{-1}$) and systematic “observed-calculated” deviations caused by “diagonal” parameters incorrectness, and especially large deviations (up to $0.5\ \text{cm}^{-1}$) for highly excited perturbed energy levels. The standard deviation of the calculation was $0.05000\ \text{cm}^{-1}$ compared to our $0.00052\ \text{cm}^{-1}$ rms. One conclusion drawn from this comparison is that using a large number of adjusted parameters (80 for 350 energy levels) in Ref.[10] led to the decrease of the predictive ability of the model. We also found that their fitted constants did not permit a good fit for our intensity data. To

achieve our goals, we had independently made different analysis decisions to model our positions and intensities through a higher range of J and K_a .

V.4 Second Triad Intensities.

No intensity measurements were done previously for the 2nd triad. The rotational and coupling constants in **Table 3** were used in the wavefunction calculations. The experimental line intensities shown in **Appendix 111** (236 for v_2+v_3 band, 201 for v_1+v_2 band and 89 for $3v_2$ band) were fitted with an rms value of 2.5% to determine the 11 constants of the transformed transition moment operator presented in **Table 6** (with 68% confidence intervals).

Surprisingly, only 11 parameters were needed to reproduce 526 line intensities, whereas 19 parameters were used for the first triad to reproduce 568 line intensities. We used 3 times less parameters for combination bands for nearly the same number of intensities as for fundamentals. In contrast, we fitted 5 parameters to reproduce 89 $3v_2$ band intensities in comparison with 6 parameters and 168 intensities for $2v_2$ band. This occurred for several reasons. First, despite the strong mixing discussed previously, few intensity anomalies were found in the second triad line intensities. In contrast, some $\Delta K_a = \pm 2$ transitions at low J in v_3 were stronger than $\Delta K_a = 0$ transitions, and additional fitted parameters were required to model this. For all three second triad vibrational bands, the main terms in the obtained parameters set are at least 30-100 times larger than the others. Secondly, the experimental intensities sets for the first and second triad, while similar in number of lines, contained different types of transitions. There were considerably more transitions with $\Delta K_a = \pm 3$ for VI and $2v_2$ bands in the first triad intensity set than for the v_1+v_2 and $3v_2$ bands. There are also more high K_a transitions in the first triad than the second. As mentioned above, introducing additional resonance parameters into the “rotational” fitting greatly influenced the intensity fitting for weak $3v_2$ band. Small additional cross terms between (011) and (030) states in the wave functions led to intensity borrowing from the very strong v_2+v_3 band to very weak $3v_2$ band, so some $3v_2$ line intensities were additionally perturbed. In the analysis, the rotational and coupling parameters set was checked at every new step of fitting against the corresponding intensity calculations. Finally, it was found that the selected set of rotational parameters in **Table 3** allowed

us to reproduce the $3\nu_2$ intensities without loss of accuracy, provided one more parameter (number 8) was introduced into the intensity fitting. The data set for $3\nu_2$ band, although smaller than the $2\nu_2$ data set, included several different types of transitions; those with high K_a equal to 5,6,7 required additional parameters to be adjusted, despite the fact that only a few of these transitions were measured. To a large extent, the strong resonance interactions between the (030) state and other members of triad made it necessary to use more parameters to fit its intensities.

Using the retrieved parameters in Table IS, the first and second derivatives of the dipole moment with respect to dimensionless normal coordinates were obtained using the equations of Ref. 19. For the input constants, the enharmonic force field was taken from Halonen et al.³⁶, assuming a dipole moment of -0.974 D as in Ref. 9, but we used our own values for C (=4.83 cm⁻¹) and ξ_{23}^y (= -0.9898). Dipole moment derivatives obtained are presented in **Table 8** along with the ab initio estimations of Senekowitch et al. [32]. For comparison, the previous first derivatives of dipole moments are also listed; these are based on the experimental results of Lechuga-Fossat et al. [9] from ν_1 and ν_3 and Camy-Peyret et al.. [22] from ν_2 .

In their paper, Senekowitch et al. have assumed a positive sign for the permanent dipole moment, and so all their derivatives must be taken with opposite signs. As seen from the **Table S**, there is rather poor agreement between two of the observed and calculated first derivatives, but agreement for two of the second derivatives is nearly within the experimental uncertainties. The calculation correctly predicts that some second order derivatives are larger than the first order ones. While it is well known that only the relative signs of the dipole moment parameters are obtained in fitting intensities, different choices of their signs leads to a worse disagreement between the ab initio and experimental results. The same solution for the intensity fitting can be obtained, when leading terms in the transition moment operator parameters are negative for all second triad bands, but in this case the second derivatives do not correlate with the ab initio estimations. The observed disagreement in $\partial\mu_x/\partial q_i$ values was discussed by Senekowitch et al., but his speculation as to the cause for this seems to be incorrect; it is clear that the differences between observed and ab initio band intensities of VI and ν_3 are not caused by ambiguities in past assignments [9] because of resonance mixing. In any case, as seen in **Table 9**, the sum of integrated intensities of VI and ν_3 is not equal to sum of ab initio estimations, as expected. Clearly, further investigation into the H₂S

dipole moment function is needed.

V.5 The molecular database of hydrogen sulfide from 2150 to 4260 cm⁻¹

The analysis of the main isotope transitions alone did not provide complete knowledge of the absorption H₂S spectrum because of the presence of isotopic and hot band transitions. Thus in order to provide a reliable molecular database, the intensities of these other bands were computed and compared with a more limited set of measurements. The intensities of the H₂³⁴S and H₂³³S lines of the first and the second triad were calculated in the same manner as in Ref.[9] using the corresponding rotational wavefunctions based on constants given in **Tables 4 and 5** and the H₂³²S transition moment parameters in **Table 6**. Calculated intensities were multiplied by the corresponding isotopic abundance (0.95, 0.0422, 0.0078). The hot bands intensities were calculated in accordance with Eq. (7), where it is assumed that:

$|i\rangle = \sum_K C_{JK}^{(010)} |010\rangle |JKT\rangle$, $|f\rangle = \sum_{VK} C_{JK}^V |V\rangle |JKT\rangle$ and $|V\rangle = |011\rangle, |110\rangle, |030\rangle$ for the 1st triad hot bands, or $|V\rangle = |1021\rangle, |1120\rangle, |040\rangle$ for the 2nd triad hot bands; the dipole moment matrix element was approximated as follows:

$$\langle i|\mu_z'|f\rangle = \sum_v \sqrt{V_2} \sum_{KK'} C_{JK}^{(010)} C_{JK'}^V \left\langle JKT \left| \sum_{j=1}^8 \mu_j' v_j A_j \right| JK'T' \right\rangle \quad (12)$$

In Eq. (12), $v = (v_1, v_2, v_3)$, $v' = (v_1, v_2 - 1, v_3)$ and μ_j' are known cold bands parameters for 1st and 2nd triads.

In the first triad region, 219 lines (including doublets) were assigned to the $3v_2 - v_2$, $v_1 + v_2 - V_2$ and $v_2 + v_3 - v_2$ bands. In the second triad interval, 411 transitions (including doublets:) were attributed to three hot bands near 2.7 pm: 42 lines for $4v_2 - v_2$, 192 lines for $2v_2 + v_3 - v_2$ and 177 lines for $v_1 + 2v_2 - V_2$. The observed -calculated intensities ranged from 2 to 15% with rms values around 6%

The integral band intensities of all analyzed bands of H₂³²S, H₂³³S, H₂³⁴S in the first and

second triad regions are presented in **Table 9**. The integral band intensities have been calculated as a sum of individual line intensities greater than the weakest observed lines in the analyzed spectrum in the spectral region from 2150 to 3000 cm⁻¹ and 3300-4260 cm⁻¹. The first triad region consisted of 6563 lines (3803, 1568 and 713 lines for H₂³²S, H₂³⁴S, H₂³³S of the first triad and 479 hot band lines). The second triad region contained 4446, 2514, 1697 lines for H₂³²S, H₂³⁴S, H₂³³S, respectively and 1511 hot band lines. The line positions where possible were calculated from the experimental energy levels in order not to decrease the accuracy of the calculation.

In **Table 9**, the ab initio estimations of Senekowitch are also presented for comparison. Our integrated band intensities for v₁, v₃ and 2v₂ bands differ by factors of 0.32, 0.90 and 1.08 respectively from Senekowitch calculation.

Conclusions

The absorption spectrum of H₂³²S, H₂³³S and H₂³⁴S between 2150 and 4260 cm⁻¹ spectral region is now well understood. Reliable rotational, resonance coupling and transition moment operator parameters are available from the fits of experimental energy levels and line intensities. The intensities of the combination bands of the second triad are seen to be larger than the fundamentals of the first triad. The fitted parameters permit the experimental data to be reproduced close to the experimental uncertainties of the line centers (0.0004 -0.0006 cm⁻¹) and well within experimental precision for line intensities (2.5%). Because the intensity fitting depends so strongly on the vibrationally-mixed rotational wave functions, it is very helpful to let the choice of theoretical model for the energies be determined by how well the intensities fit.

The molecular database for H₂S molecule between 2150 and 4260 cm⁻¹ is available in the 1997 GEISA databank (37). Experimental second order dipole moment derivatives are obtained for the first time, and previous measurements of two first derivative dipole moments are validated. The previous conclusion is confirmed that the H₂S dipole moment function can not be approximated by a linear expansion, and additional study is needed to model these data.

Questions remain concerning what is the best Hamiltonian formulation for hydrogen sulfide. Recent studies of its ground state have been successful in modeling very accurate frequency measurements of more limited values of J and K_a , but these studies do not extrapolate well to the highest quantum numbers observed in the present study. A future simultaneous fitting of all prior data together with combination differences from the first and second triads might provide a rigorous test of this question. For the higher vibrational states, the need to increase the number and values of the higher order centrifugal distortion terms is a symptom of a less-than-satisfactory situation with the modeling. The parameters, when used in such abnormally high numbers, become no more than adjustable values without any predictive capabilities. Our ongoing studies of the higher H_2S polyads may reveal sharper deterioration of the theory. Therefore, with all our qualms about the status of the theory, it is very pleasing that the model for intensities is working so well.

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Summary of Tables

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Figures Captions

Figure 1 The broadband spectrum in the regions of the first and second triads of hydrogen sulfide. The path is 0.25 m with the hydrogen sulfide pressure of 40. Torr at 288.8 K. The spectrum also contains features arising from CO near 2140, CO₂ near 2340 en]^{*} and H₂O between 3100 - 4100 cm⁻¹.

Figure 2 Example of measurement of line position, intensities and widths by non-linear least squares curve-fitting. In the lower panel, the observed and synthetic spectra are overlaid. in the upper panel, the differences between the observed and computed are shown to ± 0.5 %. The path is 0.25 m with the hydrogen sulfide pressure of 18. Torr at 288.9 K. The feature at 3717.81cm⁻¹ is a residual water line.

Appendices

- I Vibrational energy levels of the (01 1), (1 10) and (030) of H₂S (in cm⁻¹)
- II Observed Intensities of the 1st Triad of Hydrogen Sulfide
- III Observed Intensities of the 2nd Triad of Hydrogen Sulfide

TABLE 1 EXPERIMENTAL CONDITIONS OF H₂S LABORATORY SPECTRA⁺

BAND PASS (cm-')	PRES. Torr	PATH Meter	TEMP K	Posi tions Calib Ref.
848.5 - 2756.8	14.00	1.50	295.7	24
848.5 - 2756.8	31.40	1.50	296.0	24
1850.0 - 5240.2	3.00	0.25	292.4	23
1850.0 - 5240.2	7.00	0.25	289.7	23
1850.0 - 5240.2	18.00	0.25	288.9	23
1850.0 - 5240.2	40.00	0.25	288.8	23
1850.0 - 5240.2	90.00	0.25	288.8	23
1850.2 - 5246.0	1.49	16.40	292.1	x 25
1850.2 - 5246.0	3.39	16.40	289.7	
1850.2 - 5246.0	9.99	16.40	289.6	
1850.2 - 5246.0	9.99	28.20	289.3	x 26
2979.7 - 8822.2	4.80	25.0	296.5	x 26
2974.9 - 8822.2	9.99	28.4	289.2	
2977.6 - 8820.7	4.60	433.0	297.0	x 26

⁺ The first two spectra were recorded at 0.0056 cm-' resolution; the others were recorded at 0.011 cm-' resolution.

TABLE 2 Number of H₂S upper state levels and transition intensities fitted

Band	Center cm ⁻¹	I so	# E'	J' max	K' Max	rms cm ⁻¹	# Inten.	J' max	K' max	% rms
2v ₂	2353. 96	32		227	19	14	0. 00047			
	2352. 87	33		69	13	9	0. 00064			
	2351. 83	34		130	15	11	0. 00045			
v ₁	2614. 41	32		259	20	14	0. 00039			
	2613. 35	33		87	15	9	0. 00054			
	2612. 36	34		156	16	11	0. 00043			
v ₃	2628. 45	32		237	19	13	0. 00038			
	2627. 25	33		23	9	8	0. 00080			
	2626. 12	34		91	14	9	0. 00056			
3 v ₂	3513. 79	32		146	14	12	0. 00050			
	3512. 16	33		12	8	3	0. 00039			
	3510. 63	34		60	10	6	0. 00040			
v ₁ +v ₂	3779. 77	32		297	20	15	0. 00054			
	3777. 58	33		119	15	10	0. 00045			
	3776. 09	34		183	18	13	0. 00039			
v ₂ +v ₃	3789. 27	32		307	20	15	0. 00050			
	3787. 53	33		126	16	10	0. 00044			
	3785. 90	34		201	18	13	0. 00038			

+ #E' is the number of upper state levels fitted; #intens. is the number of intensities.

Table 3 The fitted parameters (in cm⁻¹) for the first and second triads of H₂³²S

	(001)	(100)	(020)	(011)	(110)	(030)
E	2628. 4545110(1300)	2614. 4085440 (1200)	2353. 9646840 (1400)	3789. 2692120 (1600)	3779. 1664600 (1600)	3513. 7901080 (2100)
A	10. 14345062(3000)	10. 20121325 (2400)	11. 11408795(2600)	10. 49043484 (3200)	10. 55640904 (3200)	11. 54035144 (4800)
B	8. 93844052(2600)	8. 89365462 (2400)	9. 44627863(1800)	9. 14751204 (2400)	9. 10066739 (2200)	9. 68616443(3500)
C	4. 67714581(3200)	4. 660670553(8200)	4. 60765546(3100)	4. 616251243(9300)	4. 598508633(9100)	4. 54552034(1800)
Δ_k	X10 ²	0. 36593509(8400)	0. 36469987 (7100)	0. 5621785 (1200)	0. 4492100 (1100)	0. 4485305 (1100)
Δ_{ik}	X10 ²	-0. 23071917(5300)	-0. 22535859 (5300)	-0. 32901690(9300)	-0. 27671468 (8400)	-0. 26989617 (9300)
Δ_j	X10 ³	0. 6628301 (1400)	0. 6454313 (1200)	0. 8809970 (1800)	0. 7686192 (1600)	0. 7487967 (1400)
δ_k	X10 ⁴	-1. 377485 (2900)	-1. 315829 (2400)	1. 221990 (3100)	-0. 346489 (2900)	-0. 217746 (2700)
δ_j	X10 ³	0. 30045643(8000)	0. 29212282 (6900)	0. 40983187(9800)	0. 35355724 (9400)	0. 3419179 (2000)
H _k	X10 ⁵	0. 133528 (1400)	0. 1412083 (8700)	0. 455276 (2200)	0. 255250 (1800)	0. 261730 (1700)
H _{ij}	X10 ⁶	1. 19572 (1300)	1. 05639 (1100)	0. 49084 (1900)	0. 95312 (1800)	0. 92804 (1700)
H _{jk}	x10 ⁵	-0. 1524165 (4700)	-0. 1446575 (4400)	-0. 2317344 (8700)	-0. 1874723 (6100)	-0. 1795210 (7900)
H _i	X10 ⁶	0. 2753521 (7800)	0. 2671332 (7000)	0. 506367 (1000)	0. 374842 (1000)	0. 357942 (1300)
h _k	X10 ⁵	0. 1165000 (5000)	0. 1187406 (3000)	0. 3440503 (5900)	0. 2055804 (6000)	0. 2117244 (5900)
h _{jk}	x10 ⁶	-0. 477294 (2800)	-0. 434553 (2600)	-0. 843633 (4300)	-0. 650889 (2900)	-0. 613937 (2700)
h _j	x10 ⁶	0. 1370370 (4300)	0. 1336931 (3700)	0. 2536025 (5700)	0. 1888030 (4800)	0. 1782055 (7100)
L _k	X10 ⁸	-0. 328783 (4200)	-0. 367750 (3400)	-1. 87187 (1600)	-0. 90806 (1200)	-0. 84919 (1200)
L _{kkj}	x10 ⁸	0. 393754 (6400)	0. 444972 (7100)	2. 27863 (1800)	1. 15102 (1100)	1. 07259 (1100)
L _{jk}	X10 ⁸	-0. 234968 (5400)	-0. 238141 (5600)	-1. 03252 (1400)	-0. 580897 (6300)	-0. 584506 (6200)
L _{ijk}	x10 ⁹	0. 88910 (1400)	0. 90123 (1500)	2. 38399 (3000)	1. 56093 (1600)	1. 51581 (2200)
L _j	x10 ⁹	-0. 127278 (1200)	-0. 127913 (1000)	-0. 314052 (1700)	-0. 193458 (1600)	-0. 182164 (2700)
t _k	X10 ⁶	-0. 114917 (1500)	-0. 125240 (1300)	-0. 938637 (7500)	-0. 453849 (5500)	-0. 491849 (5500)
t _{kj}	X10 ⁹	-0. 35580 (2200)	-0. 35358 (1600)		-0. 207129 (1300)	-0. 13538 (1200)
t _{jk}	x10 ⁹	0. 291310 (8800)	0. 275327 (8700)	0. 71741 (1500)	0. 536098 (8500)	0. 523132 (8300)
t _j	x10 ¹⁰	-0. 633841 (7100)	-0. 646428 (5500)	-1. 590498 (9100)	-0. 981961 (8500)	-0. 92032 (1400)
P _k	x10 ¹⁰			0. 38226 (1000)	0. 235537 (4400)	0. 214734 (4400)
P _{kkj}	x10 ¹⁰			-0. 52113 (1900)	-0. 348031 (5700)	-0. 326115 (5900)
P _{kj}	x10 ¹⁰			0. 174543 (9700)	0. 125290 (2700)	0. 128077 (3000)
P _k	x10 ¹¹			1. 77738 (2700)	0. 76892 (1900)	0. 84942 (1800)
P _{kkj}	x10 ¹¹			-0. 26579 (1400)		4. 5342 (1700)
<u>Coupling constants</u>						
c_x		0. 000084383(1800)				
c_y		0. 01445389 (9300)	(100)-(001)		c_y	-0. 0751971 (4000)
c_{xz}		-0. 14441749 (8200)			c_{xz}	-0. 15099194 (6200)
c_K		-0. 00267237 (2300)			c_z	0. 00184218 (5300)
c_{x^2}		0. 0299531 (1200)	(020)-(001)		c_{xz}	0. 0377344 (5200)
c_y		0. 39460 (1000)			c_{xzJ}	-0. 0000309048(8200) (030)-(011)
K		0. 0037577 (1400)	(020)-(100)		c_z	-0. 00066787 (3600)
					c_{xzK}	0. 00001 66567(4600)
					F_J	0. 0305831 (3300) (030)-(110)
					F_{xyK}	0. 0000306439(4800)
<u>Coupling constants</u>						

RMS = 0.00041 cm⁻¹ with 86 parameters (79 **diagonal** + 7 coupling)
The quoted errors are one standard deviation.

RMS= 0. 00052 cm⁻¹ with **94** parameters (85 **diagonal** + 9 **coupling**)

Table 4 The fitted parameters (in cm⁻¹) for the first and second triads of H₂³⁴S

	(001)	(100)	(020)	(011)	(110)	(030)
E	2626.1195640 (1700)	2612.3624160 (1300)	2351.8372720 (1400)	3785.8993640 (1000)	3776.0894400 (1100)	3510.6261680 (1400)
A	10.10902177 (2800)	10.16509930 (2500)	11.07533755 (1700)	10.45479071 (1800)	10.51895843 (2000)	11.50009099 (4000)
B	8.93798972 (2200)	8.89424256 (1800)	9.44522829 (1200)	9.14660974 (1800)	9.10083626 (1900)	9.68473196 (2200)
C	4.669498581 (7500)	4.653350680 (7200)	4.600323850 (4600)	4.60875601 (29200)	4.591326852 (9500)	4.538380728 (7400)
Δ_k	X10 ² 0.36447608 (8200)	0.36298208 (5100)	0.55943976 (5800)	0.44715786 (3500)	0.44652466 (4500)	0.6926497 (2000)
Δ_{jk}	X10 ⁰ -0.23036189 (3400)	-0.22515996 (3500)	-0.32872506 (4200)	-0.27620038 (3200)	-0.26980192 (5000)	-0.3955960 (1300)
Δ_i	X10 ¹ 0.66224315 (7800)	0.64539010 (4700)	0.88058523 (6600)	0.76782330 (5600)	0.7487532 (1300)	1.0293686 (2800)
δ_k	X10 ⁰ -1.4180355 (9900)	-1.349006 (1000)	1.1556057 (8700)	-0.400809 (1500)	-0.266567 (1400)	3.099109 (5000)
δ_j	X10 ⁰ 0.30036967 (4200)	0.29215078 (2100)	0.40986977 (3000)	0.35342215 (3100)	0.34203383 (5200)	0.4854921 (1300)
h_k	X10 ⁵ 0.1345251 (6100)	0.1395862 (2500)	0.4472338 (6300)	0.2510664 (4100)	0.2587608 (4000)	0.742673 (2600)
h_{kj}	X10 ⁰ 1.200	1.060	0.549580 (6700)	0.984804 (5200)	0.941222 (5200)	
h_{jk}	X10 ⁵ -0.1527	-0.14485460 (8500)	-0.2336411 (2700)	-0.1878503 (1600)	-0.1798699 (2700)	-0.2855
h_i	X10 ⁰ 0.2757	0.2675	0.5070	0.3739948 (1300)	0.3590414 (4600)	0.6542
h_k	X10 ⁵ 0.1157	0.1179	0.3417	0.2044744 (1400)	0.2107184 (1600)	0.5425
h_{jk}	X10 ⁶ -0.4786	-0.4357	-0.8459	-0.6555917 (9400)	-0.614167 (1000)	-1.249
h_i	X10 ⁶ 0.1373	0.1339	0.2541	0.18865280 (7000)	0.1786133 (2435)	0.3277
L_k	X10 ⁸ -0.3288	-0.3678	-1.872	-0.9081	-0.8492	-3.956
L_{kkj}	X10 ⁸ 0.3938	0.4450	2.279	1.151	1.073	4.946
L_{jk}	X10 ⁸ -0.2350	-0.2381	-1.033	-0.5809	-0.5845	-2.382
L_{jjk}	X10 ⁰ 0.8891	0.9012	2.384	1.561	1.516	3.996
L_j	X10 ⁰ -0.1273	-0.1279	-0.3141	-0.1935	-0.1822	-0.2846
L_k	X10 ⁸ -0.1149	-0.1252	-0.9386	-0.4538	-0.4918	-1.866
L_{kj}	X10 ⁹ -0.3558	-0.3536	-0.2071	-0.2071	-0.1354	
L_{ik}	X10 ⁹ 0.2913	0.2753	0.7174	0.5361	0.5231	1.733
L_i	X10 ¹⁰ -0.6338	-0.6464	-1.590	-0.9820	-0.9203	-1.509
P_k	X10 ¹⁰		0.3823	0.2355	0.2147	1.552
P_{kkj}	X10 ¹⁰		-0.5211	-0.3480	-0.3261	-2.243
P_{kj}	X10 ¹⁰		0.1745	0.1253	0.1281	0.8428
P_k	X10 ¹¹		1.777	0.7689	0.8494	4.534
P_{kkj}	X10 ¹¹		-0.2658			
<u>Coupling constants</u>						
c_{yK}	0.000084383			c_y	0.0935813 (4400)	(110)-(011)
c_y	0.0611886 (6800)	(100)-(001)		c_{xz}	-0.15064325 (7200)	
c_{xz}	-0.14372595 (6800)					
c_y	0.3946			c_{yJ}	0.00066787	
c_{xz}	0.02981695 (4000)	(020)-(001)		c_{xz}	0.0327486 (2600)	
c_{yK}	-0.00267237			c_{yK}	-0.00191884 (2200)	(030)-(011)
c_{yK}	0.0037577	(020)-(100)		c_{xzJ}	-0.000309048	
c_{yK}				c_{xzK}	0.0000166567	
c_{yK}				c_{yJ}	0.0295204 (4400)	(030)-(110)
c_{yK}				F_{XYK}	0.00001 269785 (7600)	
<u>Coupling constants</u>						

 RMS = 0.00047 cm⁻¹ 36 parameters (33 diagonal + 3 coupling)

 RMS = 0.00039 cm⁻¹ 48 parameters (42 diagonal + 6 coupling)

 The quoted errors are one standard deviation. The parameters without errors have been fixed to the corresponding values of H₂³²S.

Table 5 The fitted parameters (in cm⁻¹) for the first and second triads of H₂³³S

	(001)	(100)	(020)	(011)	(110)	(030)
E	2627. 2493380 (5800)	2613. 3532540 (2200)	2352. 8687730 (2300)	3787. 5320150 (1500)	3777. 5800010 (1700)	3512. 1598700 (2800)
A	10. 12552945(4200)	10. 18232787(3200)	11. 09413049 (2100)	10 . 47204449(2900)	10. 53704505(2900)	11. 51916935 (7300)
B	8 . 93849167(2900)	8. 89415754(3700)	9. 44576246 (1200)	9. 14705694(2000)	9. 10076770(2200)	9. 68560970 (6900)
c	4. 67308302(1100)	4. 65693497(1000)	4 . 603820621(7500)	4. 61232305(1000)	4. 59480220(1300)	4. 541822300(8800)
Δ_k	X10 ²	0. 3652	0. 36405182(4400)	0. 56065165 (9200)	0. 44828067(7100)	0. 44744707(7200)
Δ_{ik}	X10 ⁰	-0. 2307	-0. 22556210(5600)	-0. 32851506 (9100)	-0. 27644362(3500)	-0. 26987830(4500)
Δ_j	X10 ⁰	0. 6627	0. 6457394 (1400)	0. 88057932 (3900)	0. 76796954(5800)	0. 7492528 (1400)
δ_k	X10 ⁰	-1. 398	-1. 335	1. 201502 (4400)	-0. 3687575 (9900)	-0. 243476 (1400)
δ_j	X10 ⁰	0. 3005	0. 29231192(7100)	0. 4099	0. 35352123(1500)	0. 34197753(3300)
ϵ_k	X10 ⁰	0. 1335	0. 1412	0. 4553	0. 2533300 (6300)	0' . 2604122 (6500)
H _{kj}	X10 ⁰	1. 196	1. 056	0. 4908	0. 975322 (5200)	0. 921215 (5700)
H _{jk}	x10 ⁵	-0. 1524	-0. 1447	-0. 2317	-0. 1875	-0. 1795
H _j	X10 ⁰	0. 2754	0. 267?	0. 5064	0. 3739244 (1200)	0. 3583640 (2100)
h _k	X10 ⁰	0. 1165	0. 1187	0. 3441	0. 2056	0. 5463
h _{jk}	X10 ⁰	-0. 4773	-0. 4346	-0. 8436	-0. 6509	-0. 6139
h _j	X10 ⁰	0. 1370	0. 1337	0. 2536	0. 1888	0. 1782
L _k	X10 ⁰	-0. 3288	-0. 3678	-1. 872	-0. 9081	-0. 8492
L _{kkj}	X10 ⁰	0. 3938	0. 4450	2. 279	01. 151	1. 073
L _{jk}	X10 ⁰	-0. 2350	-0. 2381	-1. 033	-0. 5809	-0. 5845
L _{jk}	X10 ⁰	0. 8891	0. 9012		01. 561	1. 516
L _j	x10 ⁹	-0. 1273	-0. 1279	-0. 314	-0. 1935	-0. 1822
L _k	X10 ⁰	-0. 1149	-0. 1252	-0. 9386	-0. 4538	-0. 4918
L _{kj}	x10 ⁰	-0. 3558	-0. 3536		-0. 2071	-0. 1354
L _{jk}	x10 ⁹	0. 2913	0. 2753	0. 7174	0. 5361	0. 5231
L _j	x10 ¹⁰	-0. 6338	-0. 6464	-1. 590	-0. 9820	0. 9203
P _k	x10 ¹⁰			0. 3823	0. 2355	0. 2147
P _{kkj}	x10 ¹⁰			-0. 5211	-0. 3480	-0. 3261
P _{kj}	x10 ¹⁰			0. 1745	0. 1253	0. 1281
P _k	x10 ¹¹			1. 777	0. 7689	0. 8494
P _{kkj}	x10 ¹¹			-0. 2658		4. 534
<u>Coupling constants</u>						
C _K	0. 000084383					
C _y	0. 060642 (1100)	(100)-(001)				
C _{xz}	-0. 1447989(1000)					
C _y	0. 3946	(200)-(001)				
C _K	-0. 00267237					
C _{xz}	0. 024240(1600)					
F _K	0. 0037577	(200)-(100)				
<u>Coupling constants</u>						
C _y	0. 0856335 (5600)					
C _{xz}	-0. 15095915(9000)					
C _y	0. 000166787					
C _K	-0. 00184218					
C _{xz}	0. 03151145(7400)					
C _{xzj}	-0. 00001309048					
C _{xzk}	0. 0000166567					
F _j	0. 0320871(4000)					
F _{xyK}	0. 0000306439					

RMS = 0.00062 cm⁻¹ 23 parameters (20 **diagonal** + 3 **coupling**) RMS = 0.00087 cm⁻¹ 23 parameters (20 **diagonal** + 4 **coupling**)
 Note. The quoted errors are one standard deviation. Parameters **without** errors have been fixed to the corresponding values of H₂³³S

Table 6 Transition moments for the H₂³²S Triads in units of 10⁻⁴ Debye

N	(001)		(100)		(020)		(011)		(110)		(030)
	This work	Lechuga et al.	This work	Lechuga et al.	This work	Lechuga et al.	This work	This work	This work	This work	This work
1	2. 193 (130)	2. 137	29. 383 (120)	29. 494	-34. 770 (150)	-34. 62	88. 751 (160)	68. 306 (140)	10. 0671(440)		
2	0. 04967(130)	0. 05155	0. 041 31(140)	0. 02447	0. 01236(180)						
3	-0. 19355(290)	-0. 019138	-0. 09536(360)	-0. 10683	-0. 04314(380)	-0. 0426					-0. 01466(190)
4	-2. 6447 (130)	-2. 4796	3. 1033 (180)	2. 9830	-1. 4108 (150)	-1. 223	0. 1389(260)	0. 4584(150)	-0. 28593(710)		
5		-0. 01176	-1. 4283 (220)	-1. 4191	-0. 2675 (120)	-0. 2606		0. 2287(170)	0. 05333(320)		
6	3. 3668 (140)	3.1544	-0. 01213(210)				0. 2913(210)				
7	0. 01048(190)		0. 02547(270)	0. 01642	0. 01890(240)						
8	0. 04824(130)	0. 04068	0. 03744(170)	0. 03619							-0. 005595(960)
RMS	2. 4%	13. 5%	2. 3%	11. 1%	2. 4%	5. 5%	2. 5%	2. 4%	2. 8%		
#lines	147		247		170		236	201	89		
564 lines (including doublets) and 21 parameters						526 lines (including doublets) and 11 parameters					
total RMS	2. 3% (this work)		10. 1% (Lechuga et al.)			total RMS= 2. 5% (this work)					

Note.

Quoted errors are one standard deviation, and the RMS is the (obs. - calc.)/calc. intensities in %

Table 7 The **most** perturbed (011), (110) and (030) energy **levels** for the certain J-value.

			mixing, %				mixing, %				mixing, %									
J	Ka	Kc	(011)		110	030	J	Ka	Kc	(110)		011	030	J	Ka	Kc	(030)		011	110
3 2 1			3898.2670		14.4	0.0	3 3 1			3895.8995		14.4	0.0							
4 3 1			3973.6993		10.7	0.0	4 4 1			3978.3958		10.7	0.0							
5 3 2			4056.4484		12.6	0.0	5 4 2			4052.6920		13.2	0.0							
6 4 2			4167.8572		25.9	0.0	6 5 2			4172.786926.9		0.0								
7 5 2			4299.9913		10.6	0.0	7 6 2			4310.8655		11.8	0.0							
8 5 3			4429.2099		48.8	0.0	8 6 3			4434.1009		50.7	0.0							
9 6 3			4597.6879		18.9	0.0	9 7 3			4607.621621.5		0.0								
10 6 4			4761.1522		26.5	0.0	10 7 4			4755.8658		28.9	0.0							
11 7 4			4960.6530		30.5	0.0	11 7 4			4950.0164		4.9	3.2							
							11 8 4			4969.383634.0		0.0								
12 8 4			5181.3663		17.8	0.1	12 5 7			5032.2643		1.4	8.0							
12 9 4			5205.2226		13.2	1.0	12 9 4			5197.4754		22.2	0.1	129 3	5032.9544	0.1	8.2			
13 1 12			4821.7140		0.6	3.7														
13 2 12			4821.7140		0.6	3.7														
13 8 5			5386.7750		44.6	0.1	1 3 9 5			5394.5431		48.7	0.2							
14 9 5			5642.2034		17.735.3		14 10 5			5656.433829.3		0.7		14 12 3	5640.852729.3	7.0				
							14	12	3	5765.7773		12.8	37.2	14141	*5768.1071	6.131.5				
							14	12	2	5765.8711		12.1	40.1	14140	*5768.1624	6.534.1				
15 9 6			5881.8431		29.0	14.7	1 5 6 9			5669.1628		2.4	6.0	15 124	*5877.7909	4.613.9				
16 8 8			6053.9047		3.0	20.8	15 10 6			5873.917943.6		3.5		16116	*6059.1358	21.1	0.4			
16 106			6162.5830		29.5	0.3	16 11 6			6175.8009		35.6	0.8							

Note. **Levels**, marked by asterisks, were the calculated ones.

Table 8 First and second dipole moment derivatives for H₂S (in Debye)

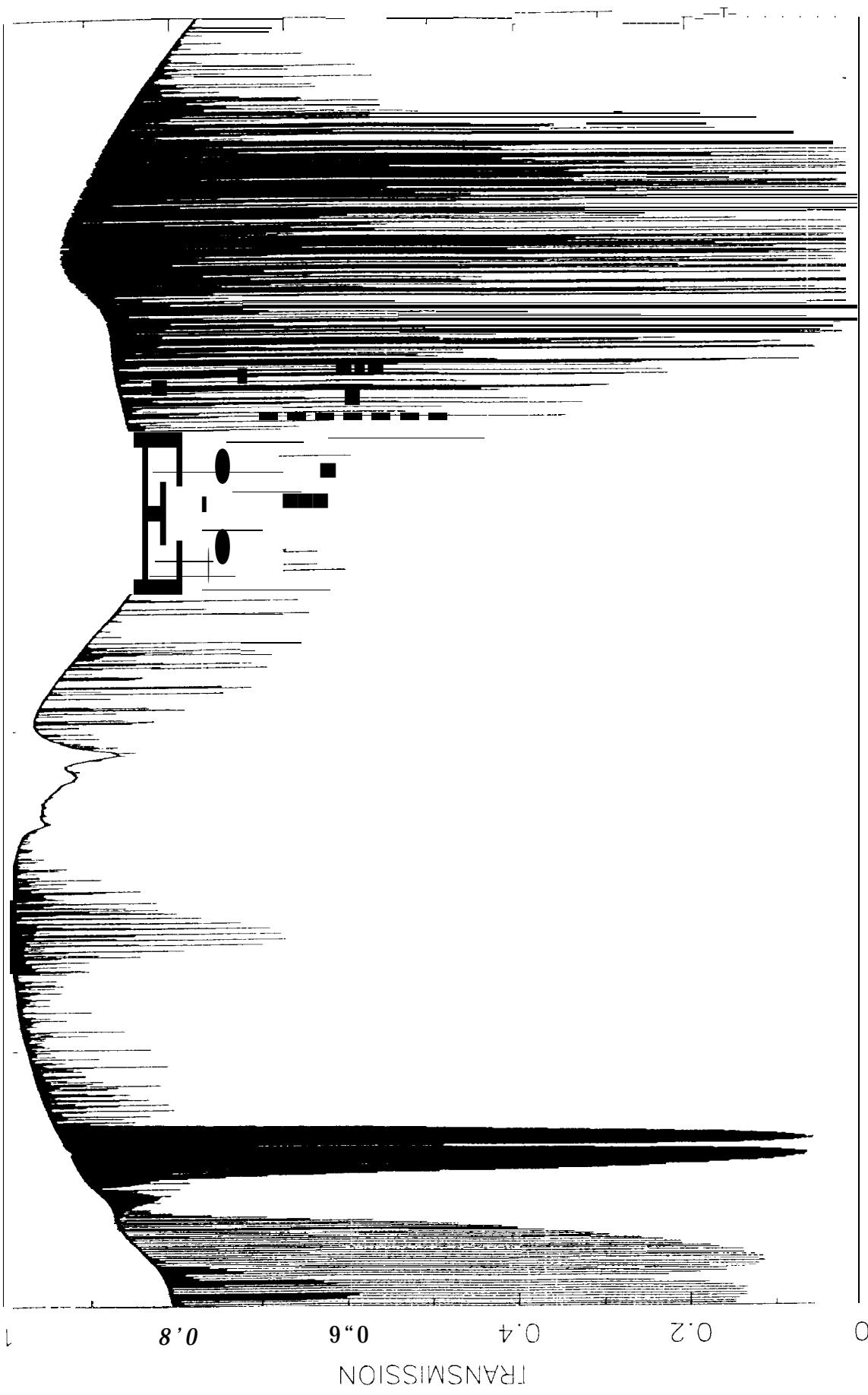
	<i>ab initio</i> [Ref. 32]	Osered Present	Observed [Ret's, 9,22]
$\partial\mu_x/\partial q_1$	0.068	-0.0041 608(96)	0.00417 I I
$\partial\mu_x/\partial q_2$	-0.027		-0.0137
$\partial\mu_z/\partial q_3$	-0.0055	0.0003036(II)	0.0003022
$\partial^2\mu_x/\partial^2q_2$	-0.0084	-0.004873(90)	-0.00492*
$\partial^2\mu_x/\partial q_1\partial q_2$	0.0140	(0.01372(30)	
$\partial^2\mu_z/\partial q_2\partial q_3$	0.0166	0.01578(30)	

* Computed using Ref. 9.

Table 9 Summary of hydrogen sulfide band intensities in natural abundances

Band (up- low)	I SO	#LINES	FMIN cm ⁻¹	FMAX cm ⁻¹ OBSERVED	INTEGRATED STRENGTHS	RAT 10 OBS/PRED
						PREDICTED	
020 000	1	?147	2142.9	2852. ?	1.337x10⁻²⁰	1. 236x10 ⁻²⁰	1. 08
001 000	1	1431	2181. 5	3024. 8	4. 843 x10 ⁻²¹	5. 371 x10⁻²⁰	0. 90
100 000	1	1225	2224. 0	3033. 3	1. 824x1 0 ⁻²⁰	5. 914 x10⁻²⁰	0. 32
020 000	2	548	2190. 6	2709. 6	5. 799x10 ⁻²²		
001 000	2	497	2327. 4	2903. 5	1. 939x10⁻²²		
100 000	2	523	2378. 9	2914. 6	7. 948 x10 ⁻²²		
020 000	3	291	2215. 1	2649. 6	9. 744 X10 ⁻²³		
001 000	3	130	2426. 5	2812. 2	2. 211X10 ⁻²³		
100 000	3	292	2467. 8	2851. 6	1. 383x1 0 ⁻²²		
030 010	1	300	2195. 3	2601. 4	1. 116 x10 ⁻²²		
011 010	1	22	2484. 8	2733. 4	3. 246x1 0 ⁻²⁴		
??0 010	1	157	2552. 9	2785. 3	4. 475 X1 0 ⁻²³		
030 000	1	853	3303. 9	4165. 2	1.221x10⁻²¹	1. 602x10 ⁻²¹	0. 76
011 000	1	?860	3384. 7	4245. 9	1.157x10⁻¹⁹	1. 549x10⁻¹⁹	0. 75
110 000	1	1733	3421. 0	4256. 6	7. 339 x10 ⁻²⁰	6. 789x10 ⁻²⁰	1. 08
011 000	2	1123	3490. 2	4157.2	5. 121 x10 ⁻²¹		
110 000	2	1025	3509. 0	4171. 8	3.263 x10⁻²¹		
030 000	2	366	3345. 0	4077. 0	5. 234x1 0 ⁻²³		
030 000	3	153	3394. 4	4024. 3	7. 653 x10 ⁻²⁴		
011 000	3	807	3551. 1	4098. 2	9. 450 X10 ⁻²²		
110 000	3	737	3570. 0	4094. 8	5.991x10⁻²²		
040 010	1	199	3326. 3	3858. 3	1. 403 X1 0 ⁻³³		
021 010	1	708	3527. 3	4060. 5	7. 076 x10 ⁻²²		
120 010	1	604	3545. 6	4063. 2	4. 461 x10 ⁻²²		

The total integrated intensity for the 24 bands included is $2.40 \times 10^{-9} \text{ cm}^{-1}/(\text{cm}^2 \times \text{molecule})$ at 296 K. For the isotopes, the intensities have been scaled by abundances of 0.950, 0.422 and 0.0078 for ^{32}S , ^{34}S and ^{33}S respectively, $\text{I}_{\text{SO}} = 1, 2, 3$. The predicted intensities are those of Senekowitch et al. scaled by the same isotopic abundances.



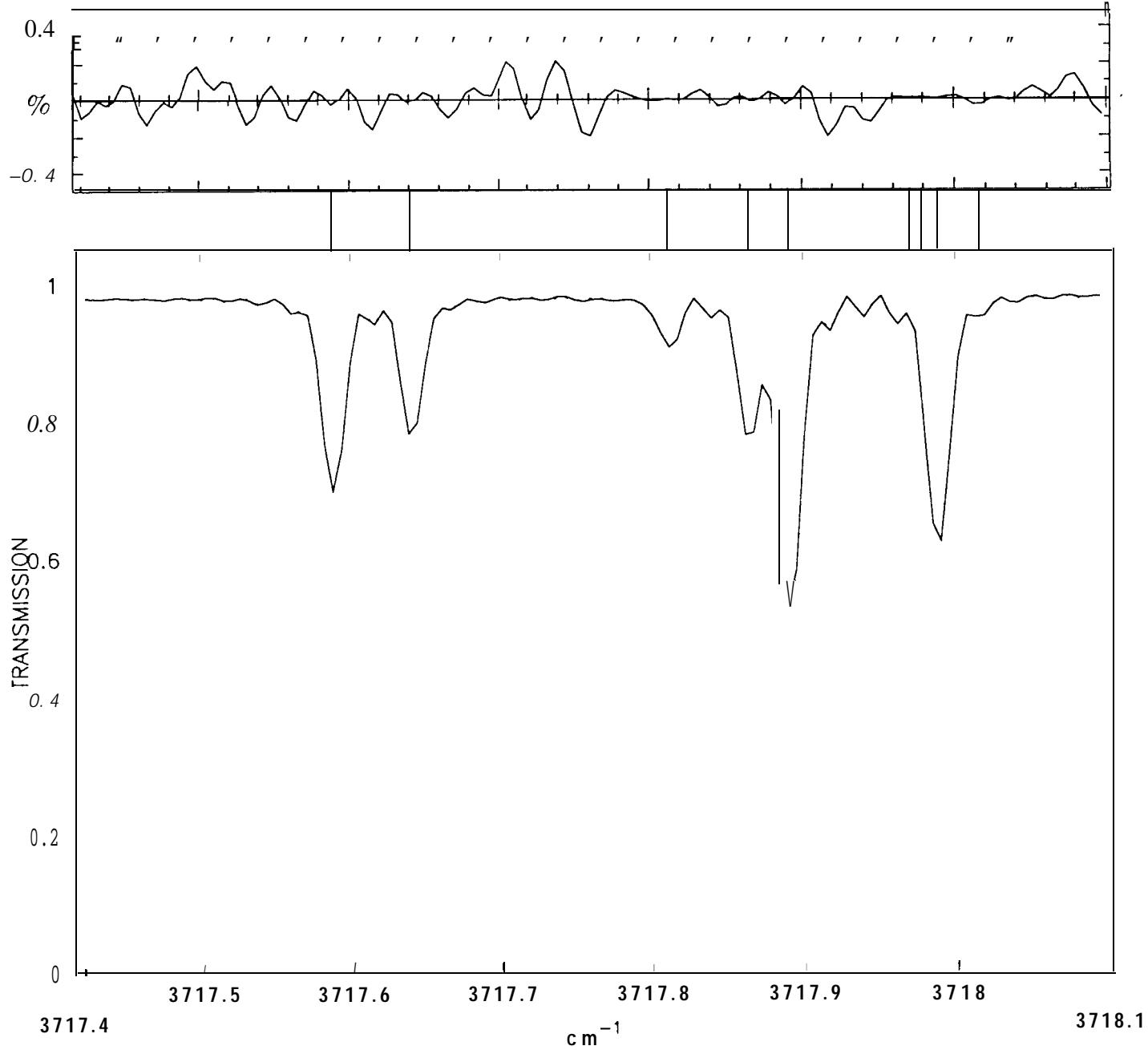
4100

cm⁻¹

2100

TRANSMISSION

HITE=0.9808 SLOPE= 0.006763 NL= 9 OK=0.21 RMS(best)= 0.000072



APPENDIX I OBSERVED UPPER STATE LEVELS OF THE SECOND TRIAD OF HYDROGEN SULFIDE

		H2S -32				H2S -34				O2S - 33																												
(01 1)		(110)		(030)		(011)		(110)		(030)		(011)		(110)		(030)		(011)		(110)		(030)																
J	K	Kc	Obs.	Obs.	E'	N	OC	Obs.	E'	E'	N	OC	Obs.	E'	E'	N	OC	Obs.	E'	N	OC	Obs.	E'	N	OC													
0	0	0	3789.2690	1	-2	3779.1665	1	0	3513.7900	1	-1	3785.8989	1	-4	37	S7	.5319	1	-1																			
1	0	1	3803.0307	1	1	3792.8582	2	0	3528.0178	2	1	3799.6518	2	-2	3789.7730	2	-2	3524.0455	2	3				3526.3830	1	-1												
1	1	1	3804.3796	2	0	3794.3196	3	-3	3529.8750	3	-3	3800.9673	2	-2	3791.1982	1	-4	3526.6636	1	-4	3802.6205	2	-1															
1	1	0	3808.9035	2	-2	3798.8200	1	-1	3535.0108	2	0	3805.4979	2	4				3531.8054	1	1	3807.1477	1	0	3797.2142	2	-2	3533.3589	1	0									
2	0	2	3827.0980	4	-1	3816.8955	1	-3	3552.7584	2	-3	3823.6753	3	1	3813.7653	1	-3	3549.5414	1	6				3815.2819	1	0												
2	1	2	3827.3505	4	-1	3817.2045	4	0	3553.1975	3	-1	3823.9170	2	1	3814.0605	2	0	3549.9634	1	0	3825.5801	2	-1				3551.5313	1	4									
2	1	1	3840.9621	3	0	3830.6774	2	1	3568.5816	3	5	3837.5436	3	-2	3827.5545	1	0	3565.3639	2	0	3839.2005	1	6	3829.0671	1	0												
2	2	1	3844.9811	3	-1	3835.0327	4	-6	3574.1295	4	-3	3041.4624	1	-1	3831.8022	2	6	3570.7970	4	2	3843.1673	2	0	3833.3670	2	0												
2	2	0	3848.4063	3	-2	3838.4170	3	-4	3577.8189	2	-3	3844.9152	1	0	3835.2125	2	0	3574.5140	1	-4				3848.1406	2	0	3584.5180	1	-1									
3	0	3	3860.0583	2	-3	3849.7853	4	0	3586.2075	4	0	3856.5786	2	-1	3846.5958	3	1	3582.9295	2	2																		
3	1	3	3860.0908	2	-5	3849.8301	2	4	3586.2798	3	-1	3856.6094	2	-1	3846.6369	1	-1	3582.9980	2	0	3858.2961	1	1															
3	1	2	3884.9444	4	0	3874.6366	1	2	3614.7573	5	4	3881.4550	4	0	3871.4444	1	-1	3611.4702	1	2	3883.1452	3	-2	3872.9906	1	-1	3613.0637	1	1									
3	2	2	3886.1539	4	0	3876.0946	4	0	3616.8082	3	1	3882.6142	4	1	3872.8400	1	0				3804.3290	2	2	3874.4167	1	3												
3	2	1	3898.2670	3	2	3887.5590	4	0	3629.6334	4	1	3894.7800	3	0	3884.3683	3	0	3626.3367	2	-3	3896.4688	2	-2	3885.9138	1	1	3627.9349	1	-1									
3	3	1	3905.9401	3	2	3895.8995	5	0	3640.5867	3	-5	3902.2629	4	-1	3892.4944	1	-2	3637.0633	1	-4	3904.0480	2	-1	3894.1435	2	-3												
3	3	0	3908.1770	3	1	3898.4377	3	-3	3642.8078	2	-1	3904.5324	3	0	3895.0696	3	-2	3639.3234	3	-1	3906.2982	1	2	3896.7008	1	-3	3641.0095	1	-1									
4	0	4	3902.1376	4	0	3891.7396	3	-1	3628.5798	1	-1	3898.5905	1	1	3888.4797	2	-2							3890.0594	2	5												
4	1	4	3902.1413	2	-1	3891.7455	3	0	3628.5907	2	-1	3898.5937	1	-2	3888.4852	1	0	3625.2416	1	-4	3900.3123	1	4	3890.0634	1	-9												
4	1	3	3937.8118	4	0	3927.5057	3	-1	3669.8521	5	4	3934.2187	3	1	3924.2056	2	1	3666.4512	2	-4	3935.9592	2	1	3925.8039	4	-2												
4	2	3	3938.0350	3	0	3927.8061	3	3	3670.3381	3	4	3934.4290	2	0	3924.4869	3	0	3666.9129	4	-:	3936.1759	1	2	3926.0945	2	1												
4	2	2	3961.3327	6	-1	3950.7584	5	1	3696.3070	2	5	3957.7715	4	0	3947.5043	3	1	3692.9462	1	2	3959.4965	2	-2	3949.0807	3	2												
4	3	2	3964.6432	4	-3	3954.6733	5	1	3701.7622	3	0	3960.9521	2	3	3951.2625	4	-3	3698.2246	4	-1	3962.7403	1	2															
4	3	1	3973.6993	3	0	3963.7633	4	0	3711.5120	2	4	3970.1155	3	3	3960.4571	2	3	3708.0827	2	4	3971.8499	1	-12															
4	4	1	3987.2966	3	0	3978.3958	3	0	3729.2481	3	-3	3983.3815	2	0	3974.7361	3	0	3725.4613	2	-1	3985.2778	3	-2	3976.5082	1	-3												
4	4	0	3988.5626	3	0	3979.2586	3	-2	3730.3990	3	-1	3984.6868	2	1	3975.6421	1	-4	3726.6465	2	3	3986.5648	1	7	3977.3933	2	-4												
5	0	5	3953.4167	2	3	3942.8533	1	6	3680.0020	1	3	3949.7084	1	1				3676.5710	1	2	3951.5454	2	5	3941.1289	1	4	3678.2330	1	-3									
5	1	5	3953.4165	2	-2	3942.8535	2	1	3680.0034	1	1	3949.7890	1	2	3939.5097	1	0				3951.5454	2	1															
5	1	4	3999.4599	5	0	3989.0616	4	0	3733.4140	4	2	3995.7613	4	2	3985.6512	1	-1	3729.8983	2	0	3997.5512	1	-11	3987.3031	3	0												
5	2	4	3999.4937	4	0	3989.1119	3	2	3733.5081	1	-2	3995.7929	1	1	3985.6980	1	3	3729.9872	1	1				3987.3511	1	-1												
5	2	3	4034.3082	4	-1	4023.8662	5	1	3773.2550	5	0	4030.5973	2	-1	4020.4570	3	0	3769.7371	3	0	4032.3948	2	-3	4022.1084	4	0												
5	3	3	4035.1627	2	4	4024.9952	6	-1	3775.0530	3	1	4031.4035	1	3	4021.5197	2	3				4033.2247	2	7	4023.2033	1	1												
5	3	2	4056.4484	5	-1	4045.1461	4	4	3797.3371	3	5	4052.7783	2	-2	4041.8124	3	0	3793.0782	2	-3	4054.5560	3	-2	4043.4273	3	4												
5	4	2	4062.9193	5	2	4052.6920	3	6	3808.1491	4	0	4059.0215	3	4	4049.0916	2	7	4056.2183	2	1	3811.1110	2	-3	4067.6722	2	3	4057.9109	1	0									
5	4	1	4069.6123	4	0	4059.7138	3	-4	3814.7546	4	-4	4065.8498	4	0	4056.2183	2	1				4067.6722	2	3	4066.8113	2	-3	4078.4187	1	-4									
5	5	1	4088.9831	3	-2	4080.4652	3	0	3840.0095	2	0	4084.7716	3	0	4076.4980	2	3	3835.8847	1	5	4066.8113	2	-3	4078.8829	1	12												
5	5	0	4089.6345	4	0	4080.9139	3	-3	3840.5492	3	3	4085.4517	3	-1	4076.9739	2	1	3836.4459	1	-1				4078.8829	1	12												
6	0	6	4013.9009	4	4	4003.1337	1	4	3740.4919	2	-3	4010.1773	2	-1	3999.6908	2	-4	3736.9647	3	1	4011.9804	1	8	4001.3577	2	-4												
6	1	6	4013.9011	2	6	4003.1329	1	-4	3740.4919	2	-3	4010.1773	2	-1				4011.9804	1	8				4057.8271	1	3												
6	1	5	4070.1987	5	5	4059.6462	2	0	3805.8515	1	2	4066.3054	3	3	4056.1183	2	3				4068.2367	1	4	4057.8347	1	3												
6	2	5	4070.2036	3	4	4059.6543	3	2	3805.8689	2	1	4066.3891	2	0	4056.1253	3	0	3802.2303	1	-2	4068.2367	1	4															
6	2	4	4115.6465	6	0	4105.2045	3	0	3858.2484	4	3	4111.7614	4	2	4101.6312	3	0	3854.5557	1	8	4113.6533	2	0	4103.3627	1	6												
6	3	4	4115.8191	4	4	4105.4455	7	4	3858.6959																													

8	4	5	4359.9846	5	1	4349.4385	5	0	4117.3132	3	-1	4355.7416	4	2	4345.4785	2	-1	4357.7969	2	4	4347.3961	4	-4						
8	4	4	4402.9280	4	-3	4391.9837	5	-6	4165.0371	1	-4	4398.7369	3	-7	4388.1219	1	-2	4400.7678	2	-2	4392.1794	2	1						
8	5	4	4404.5546	5	7	4394.2517	6	3	4169.0161	3	-3	4400.2588	5	8	4390.2331	4	3	4402.3390	1	3	4392.1794	2	1						
8	5	3	4429.2099	4	-2	4419.7826	3	-1	4196.0651	2	-6	4429.8607	4	-2	4431.9137	3	-4	4417.8799	1	-7	4427.1410	1	0						
8	6	3	4441.5520	4	0	4434.1009	4	-7	4213.0319	3	1	4437.0716	5	2	4425.1959	1	-1	4448.8877	1	0	4438.9384	1	2						
8	6	2	4451.0459	4	-5	4440.9765	2	-1	4221.5230	4	3	4446.8626	2	0	4437.0261	1	-4	4474.2778	2	-2	4466.7012	1	3						
8	7	1	4476.0027	4	-7	4469.1261	4	-1	4256.0391	3	-3	4471.9081	3	-2	4464.4230	3	-2	4475.7347	1	2	4467.6956	1	-4						
8	7	1	4478.2160	4	-2	4470.0840	3	-5	4257.0764	1	9	4473.4068	5	0	4465.4555	2	1	4505.4232	1	3	4505.4232	1	3						
8	8	1	4514.4745	2	0	4508.1629	3	9	4302.0435	1	-6	4508.9846	2	2	4502.8921	1	0	4505.4628	1	0	4505.4628	1	0						
8	8	0	4514.5426	3	0	4508.2005	2	5	4302.0878	1	-1	4509.0581	2	-1	4502.8921	1	0	4238.9066	3	-1	4236.9333	1	-3						
9	0	9	4250.5049	3	-1	4238.9066	3	0	3976.3316	3	-4	4246.4109	2	0	4235.0809	1	-3	3972.4286	1	1	4248.3913	1	-5	4236.9333	1	-3			
9	1	9	4250.5049	3	-1	4238.9066	3	0	3976.3316	3	-4	4246.4108	2	-1	4235.0809	1	-3	3972.4286	1	1	4248.3913	1	-5	4236.9333	1	-3			
9	1	8	4337.3927	3	1	4326.1392	4	2	4077.3397	2	3	4333.1549	2	-1	4322.1754	2	3	4073.2602	2	1	4335.2061	2	-3	4324.0949	2	2			
9	2	8	4337.3922	3	-2	4326.1389	3	-1	4077.3395	2	0	4333.1550	2	0	4322.1753	2	2	4073.2609	2	4	4335.2063	2	0	4324.0948	2	0			
9	2	7	4413.2580	3	3	4402.2912	5	6	4165.0021	2	7	4408.9055	3	0	4398.2160	1	-1	4400.1902	1	8	4400.1902	1	8	4400.1902	1	8			
9	3	1	4413.2582	4	-1	4402.2940	3	7	4165.0861	1	0	4408.9058	3	-2	4398.2187	1	3	4467.4611	5	-2	4463.3121	2	-2	4465.3208	1	-11			
9	3	6	4478.2217	2	3	4467.4611	5	-2	4239.8049	3	0	4473.7901	2	11	4463.3121	2	-2	4475.9361	1	3	4465.3208	1	-11	4475.9361	1	3			
9	4	6	4470.2456	4	0	4467.5023	4	1	4239.9055	2	-7	4473.8113	4	0	4463.3489	3	-4	4475.9501	2	-8	4517.1208	3	-7	4519.1321	1	-1			
9	4	5	4532.0304	3	-1	4521.2712	5	-5	4300.9264	2	-2	4527.5791	4	0	4517.1208	3	-7	4529.7354	2	-2	4530.1279	2	-1	4559.2779	1	1			
9	5	5	4532.4391	3	4	4521.8959	4	0	4302.2119	1	-1	4527.9578	4	5	4517.6938	3	-1	4564.1285	2	5	4564.1285	2	5	4564.1285	2	5			
9	5	4	4573.0635	3	-6	4561.3153	5	-4	4345.3436	3	2	4568.7217	3	-2	4557.3602	1	-6	4574.4255	3	8	4585.1651	1	2	4585.1651	1	2			
9	6	4	4576.7762	6	5	4566.3256	5	3	4374.6730	2	5	4593.5364	1	-4	4503.2929	4	1	4607.8313	3	3	4613.0362	2	7	4619.3855	2	-2	4609.9473	1	-3
9	6	3	4597.6879	2	-5	4587.1588	5	-1	4400.4063	1	9	4610.6917	4	-1	4602.9749	4	1	4620.9826	2	0	4345.5204	2	2	4333.7180	2	0			
9	7	3	4615.5323	4	-3	4607.6216	2	1	4617.1786	1	-2	4617.1786	1	-2	4607.8313	3	3	4619.3855	2	-2	4609.9473	1	-3	4609.9473	1	-3			
9	7	2	4612.7396	3	-2	4612.2054	3	-3	4405.3855	2	2	4429.0691	2	4	4181.6667	1	1	4442.4933	2	-3	4442.4934	2	-2	4442.4934	2	-2			
9	8	2	4654.2421	4	-4	4647.2147	1	3	4447.7773	1	-9	4648.8830	2	-4	4642.0195	1	-3	4528.3017	1	-5	4528.3017	1	-4	4517.2153	1	3			
9	9	1	4654.9564	3	0	4647.6750	3	-1	4440.2623	1	-9	4649.6600	2	-4	4642.5235	2	4	4692.4724	1	0	4687.2016	1	-4	4687.2194	1	5			
9	9	0	4695.5855	3	0	4690.2381	2	9	4689.5484	1	-9	4689.5484	3	5	4684.3700	1	3	4688.1427	1	-1	4688.1427	1	-1	4688.1427	1	-1			
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10	1	3	4530.6431	3	-1	4519.4148	4	0	4285.2523	1	-6	4526.1042	3	2	4515.1490	1	0	4200.0356	1	-5	4603.1547	1	2	4603.1547	1	2			
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11	1	2	9	4657.1219	5	0	4645.5939	4	-1	4414.4088	2	-3	4652.38																

1	2	3	9	4887.2377	3	1	4875.7353	2	0	4661.3235	1	5	4882.1412	3	0	4884.6137	1	7
1	2	4	9	4887.2378	2	2	4875.7352	3	-5	4661.3247	2	0	4882.1470	2	-2	4870.9140	2	1
1	2	4	8	4970.7912	3	-4	4959.5775	1	-2	4956.6013	3	0	4965.6025	2	-2	4954.6674	1	-9
1	2	5	8	4970.7932	2	0	4959.5871	2	1	4756.9547	1	1	5038.1236	3	1	5040.6642	1	-3
1	2	5	7	5043.3669	3	2	5032.2643	1	10	5032.2103	2	-3	5099.1951	2	0	5027.4759	2	-3
1	2	6	7	5043.4608	4	0	5032.4502	2	-3	5100.0151	1	-6	5089.4814	1	-2	5040.6642	1	-3
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12	11	2	5302.0868	2	0	5297.5062	2	-2	5295.0695	1	4	5290.5050	1	1	5342.1868	1	5	
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13	13	1	5607.3972	1	-2	5598.6844	1	2	5598.6844	1	2	5598.6844	1	2	5598.6844	1	2	
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1	4	8	7	5550.0534	2	-10	5539.0300	2	-6	5539.0300	2	-6	5539.0300	2	-6	5539.0300	2	-6
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14	13	1	5827.0325	1	2	5824.0992	1	17	5824.0992	1	17	5824.0992	1	17	5824.0992	1	17	
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14																		

15	2	13	5253.6168	4	2	5240.5663	3	-6
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15	14	2	6116.3560	1	-4			
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16	1	16	5122.5841	2	4	5107.7989	2	2
16	1	15	5280.2574	2	1	5266.1228	1	-3
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16	3	13	5558.3499	2	2	5545.3967	3	7
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16	5	12	5679.8616	2	10	5667.4331	3	7
16	5	11	5790.1692	2	0			
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16	6	10	5809.4598	1	5	5877.9447	1	-3
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16	13	4				6296.8340	1	-3
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17	1	16	5451.2092	2	-1	5436.5248	2	-2
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17	2	15	5605.9686	2	-8	5591.9400	2	-13
17	3	15	5605.9686	2	-8	5591.9400	2	-13
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17	4	13	5879.2671	1	0	5866.4346	1	8
17	5	13	5879.2671	1	0	5866.4345	1	7
17	5	12	5998.7400	1	0	5986.4375	2	3
17	6	12	5998.7407	1	6	5986.4371	2	-2
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18	3	16	5795.5871	1	-7			
18	3	15				5933.5077	1	0
18	4	15				5933.5877	1	0
18	4	14	6087.4674	1	-1	6074.2029	1	-5
18	5	14	6087.4674	1	-1	6074.2029	1	-5
18	5	13	6215.9916	1	1			
18	6	13	6215.9919	1	4			
19	0	19	5632.2876	2	-6	5615.6225	2	-1

19	1	19	5632.2076	2	-6	5615.6125	2	-1
19	1	18	5820.0894	1	8	5804.2059	1	9
19	2	18	5820.0893	1	7	5804.2059	1	9
19	2	17	5994.1340	1	3	5978.9976	1	-14
19	3	17	5994.1340	1	3	5978.9976	1	-14
19	3	16	6155.3504	1	-1			
19	4	16	6155.3504	1	-1			
19	4	15	6304.4337	1	-15			
19	5	15	6304.4337	1	-15			
20	0	20	5820.1490	1	3	5802.7905	1	-2
20	1	20	5820.1489	1	2	5802.7905	1	-2
20	1	19				6001.4327	2	0
20	2	19				6001.4327	2	0
20	2	18	6201.5772	1	-15	6185.8435	1	7
20	3	18	6201.5772	1	-15	6185.8436	1	8
20	3	17	6372.0439	1	18	6357.0786	1	-1
20	4	17	6372.0439	1	18	6357.0706	1	-1

++ TEE OBSERVED ENERGY IS IN CM - 1. n l S THE NUMBER OF LINE CENTERS AVERAGED TO OBTAIN THE UPPER STATE LEVEL AND OC IS THE DIFFERENCE IN OBSERVED AND CALCULATED VALUES IN 10-4 CM- 1.

APPENDIX 1 I OBSERVED INTENSITIES OF THE FIRST TRIAD OF HYDROGEN SULFIDE

I	II	III	IV	V	VI	VII	1	11	111	IV	V	VI	VII	1	11	111	IV	v	VI	VII
2216.12061	12	0 12 13 1 13	020	3.75 (4.8)	1.3	6	2397.39353	5 2 3 5 1 4	020	18.68 (2.1)	-2.3	3	2450.53074	7 2 5 6 3 4	020	18.89 (2.7)	-0.1	9		
2216.12061	12	1 12 13 0 13	020	3.75 (4. B)	1.3	6	2397.63011	3 1 2 2 2 1	020	14.28 (3.9)	1.4	9	2450.03589	7 3 5 6 2 4	020	6.58 (1.0)	3.1	4		
2222.64716	12	1 1 1 1 3 2 1 2	020	1.75 (2.5)	2.5	3	2398.05515	5 3 3 5 2 4	020	6.58 (2.9)	2.3	5	2460.53556	9 1 8 8 2 7	020	18.83 (3.4)	-1.8	6		
2222.64716	12	2 11 13 1 12	020	1.75 (2.5)	2.5	3	2390.91032	8 2 6 9 4 5	001	2.06 (4.1)	1.6	4	2460.53556	9 2 8 0 1 7	020	18.83 (3.4)	-1.8	6		
2227.11406	12	2 10 13 3 11	020	0.82 (6.2)	1.0	2	2400.06354	2 2 0 1 1 1	020	5.42 (4.1)	4.0	5	2460.63071	4 2 2 3 1 3	020	1.45 (0.2)	5.9	2		
2227.11406	12	3 10 13 2 11	020	0.82 (6.2)	1.0	2	2401.80552	6 3 3 6 2 4	020	5.12 (4.8)	-2.1	5	2461.70017	6 2 4 7 4 3	001	4.25 (3.7)	-0.1	4		
2227.63335	11	0 11 12 1 12	020	6.44 (2.3)	3.6	4	2403.43552	3 2 2 2 1 1	020	8.80 (3.0)	0.3	6	2465.45172	4 3 2 3 0 3	020	3.90 (4.1)	3.6	5		
2227.63335	11	1 11 12 0 12	020	6.44 (2.3)	3.6	4	2403.78381	5 1 4 5 0 5	020	14.78 (1.3)	1.1	9	2467.00349	6 4 3 5 3 2	020	18.50 (1.8)	-2.5	9		
2232.66768	11	1 10 1 2 2 1 1	020	2.99 (5.5)	1.3	3	2403.85852	5 2 4 5 1 5	020	5.06 (3.3)	3.6	6	2469.46423	8 2 6 7 3 5	020	4.96 (5.7)	-0.5	6		
2232.66768	11	2 10 12 1 11	020	2.99 (5.5)	1.3	3	2404.47947	6 5 2 6 4 3	020	13.46 (2.7)	-1.3	7	2469.52494	8 3 6 7 2 5	020	14.76 (2.9)	-1.6	6		
2235.77180	11	2 9 12 3 10	020	1.43 (4.0)	-1.6	4	2405.00678	7 6 1 7 5 2	020	8.00 (3.5)	-7.0	6	2472.15050	7 3 4 6 4 3	020	12.59 (1.9)	-0.3	8		
2235.77180	11	3 9 1 2 2 1 0	020	1.43 (4.0)	-1.6	4	2405.59602	6 4 3 6 3 4	020	15.45 (2.4)	-2.1	E 8	2472.32758	8 6 2 9 6 3	001	3.68 (5.4)	-6.5	2		
2238.93473	10	1 10 11 0 11	020	9.98 (2.2)	1.3	6	2406.13255	7 4 3 7 3 4	020	9.94 (2. e)	-8.6 8		2472.56063	5 5 1 4 4 0	020	17.26 (3.1)	1.5	8		
2238.93473	10	0 10 11 1 11	020	9.98 (2.2)	1.3	6	2409.74353	6 2 4 6 1 5	020	5.45 (3.9)	3.5	3	2474.25121	5 5 0 4 4 1	020	51.90 (3.0)	0.7	7		
2240.62930	6	6 1 7 7 0	020	1.92 (1.4)	3.9	3	2409.77424	6 6 1 6 5 2	020	8.32 (1.7)	2.9	5	2474.69342	6 3 3 7 5 2	001	6.26 (2.7)	0.1	5		
2250.02149	9	9 1 9 0 0 1 0	020	14.95 (2.5)	1.0	8	2410.09511	6 3 4 6 2 5	020	15.72 (1.9)	-0.8	9	2476.22296	7 4 4 6 3 3	020	5.04 (0.7)	2.3	4		
2250.02149	9	0 9 1 0 1 1 0	020	14.95 (2.5)	1.0	8	2410.74477	4 1 3 3 2 2	020	9.00 (2.6)	1.7	6	2476.51678	5 2 4 6 4 3	001	3.58 (4.7)	0.1	3		
2252.13337	9	1 6 1 0 2 9	020	7.47 (2.5)	0.1	8	2412.48593	4 2 3 3 1 2	020	28.83 (1.0)	-0.9	8	2480.11433	10 3 7 1 1 3 8	001	0.70 (7.0)	-4.3	2		
2252.13337	9	2 8 1 0 1 9	020	7.47 (2.5)	0.1	B	2413.77090	7 5 3 7 4 4	020	3.58 (3.6)	-0.2	4	2480.11433	10 4 7 11 4 8	001	0.70 (7.0)	-4.3	2		
2253.33681	5	5 0 6 6 1	020	3.71 (2.3)	-1.0	4	2414.19100	6 1 5 6 0 6	020	4.21 (5.3)	2.5	5	2400.78858	8 5 3 9 5 4	001	4.27 (4.1)	-1.9	5		
2255.33008	8	5 4 9 4 5	020	1.22 (3.7)	3.2	2	2414.20435	6 2 5 6 1 6	020	12.79 (1.9)	3.7	6	2401.33996	5 3 3 6 5 2	001	4.29 (2.1)	-0.3	5		
2258.11575	8	4 5 9 3 6	020	2.20 (5.9)	-3.0	4	2414.67322	B 5 4 9 6 3	100	0.58 (5.1)	4.2	3	2401.97678	5 3 2 4 2 3	020	8.32 (1.9)	2.8	6		
2260.58946	8	3 6 9 2 7	020	4.22 (5.5)	-1.4	4	2416.03946	7 3 4 7 2 5	020	11.43 (3.2)	-3.5	8	2405.62325	8 3 5 7 4 4	020	3.86 (1.4)	4.6	3		
2260.88980	8	0 8 9 1 9	020	21.11 (1.9)	0.5	9	2417.21619	7 4 4 7 3 5	020	4.11 (4.8)	2.9	4	2496.70149	6 5 1 5 4 2	020	8.68 (3.1)	0.9	4		
2260.88980	8	1 8 9 0 9	020	21.11 (1.9)	0.5	9	2418.19113	7 2 6 8 4 5	001	2.33 (3.4)	5.3	4	2497.00863	7 5 3 6 4 2	020	4.79 (2.9)	-0.7	5		
2261.56534	8	1 7 9 2 8	020	10.93 (1.5)	0.8	8	2418.25998	3 3 1 2 2 0	020	13.30 (2.6)	1.4	8	2497.70245	9 3 6 8 4 5	020	8.23 (3.5)	0.9	6		
2261.56534	8	2 7 9 1 8	020	10.93 (1.5)	0.8	B	2420.36545	7 7 0 7 6 1	020	4.84 (1.3)	5.0	5	2497.87011	4 0 4 5 2 3	001	1.97 (4.1)	-1.8	4		
2265.61724	4	4 1 5 5 0	020	5.82 (5.6)	-4.3	6	2421.32560	7 2 5 7 1 6	020	11.95 (2.6)	-2.4	8	2500.90138	6 6 1 5 5 0	020	46.11 (1.8)	0.0	7		
2267.33732	4	4 0 5 5 1	020	2.08 (2.7)	-4.9	3	2421.40071	7 3 5 7 2 6	020	3.97 (5.5)	-2.8	6	2501.80291	6 6 0 5 5 1	020	15.43 (3.0)	-0.5	6		
2270.78611	7	1 6 8 2 7	020	15.12 (1.9)	2.2	9	2421.70899	5 1 4 4 2 3	020	29.79 (3.5)	-1.9	9	2503.20349	7 5 3 8 5 4	001	3.09 (1.7)	2.6	3		
2270.78611	7	2 6 8 1 7	020	15.12 (1.9)	2.2	9	2422.06249	5 2 4 4 1 3	020	11.13 (2.8)	7.8	7	2503.55532	6 4 2 5 3 3	020	3.66 (3.7)	3.4	4		
2271. 02886	5	3 2 6 4 3	020	3.91 (2.7)	-5.6	5	2423.54499	8 6 3 8 5 4	020	5.92 (3.2)	-6.1	5	2505.95542	8 5 4 7 4 3	020	9.06 (2.0)	-1.3	6		
2271.53635	7	0 7 8 1 8	020	28.08 (3.9)	0.1	9	2423.63050	3 3 0 2 2 1	020	33.94 (2.9)	0.3	B	2508.22919	6 5 1 7 5 2	001	6.75 (2.3)	-0.9	6		
2271.53635	7	1 7 8 0 8	020	28.08 (3.9)	0.1	9	2425.30884	B 5 4 8 4 5	020	7.08 (4.0)	-5.1	6	2509.39983	10 3 7 9 4 6	020	1.88 (3.6)	3.1	4		
2275.15472	4	3 1 5 4 2	020	1.95 (2.5)	4.2	3	2427.55631	7 3 5 8 5 4	001	2.93 (3.7)	-2.2	5	2509.45845	10 4 7 9 3 6	020	5.74 (3.6)	4.9	5		
2276.22015	6	3 4 7 2 5	020	7.35 (3.71)	-1.9	6	2427.63414	8 7 2 8 6 3	020	4.76 (1.6)	2.5	3	251.0. BB298	4 1 3 5 3 2	001	4.45 (3.0)	-1.4	5		
2276.61025	6	5 2 7 4 3	020	1.52 (2.3)	5.2	2	2427.68197	0 4 4 9 6 3	001	2.81 (3.9)	-3.2	4	2511.10257	6 6 0 7 6 1	001	1.69 (3.9)	7.0	2		
2283.13066	3	3 0 4 4 1	020	9.57 (3.2)	-3.3	7	2420.45829	3 2 1 2 1 2	020	6.91 (2.4)	2.9	6	2512.62769	7 4 4 0 4 5	001	3.00 (2.7)	4.2	3		
2207.70351	4	2 2 5 3 3	020	2.85 (1.0)	1.6	2	2429.30704	8 4 5 8 3 6	020	8.07 (2.9)	-4.9	B	2512.68694	9 4 5 8 5 4	020	5.67 (5.1)	0.0	5		
2208.52498	5	1 4 6 2 5	020	16.08 (2.5)	-2.1	9	2429.50781	4 3 2 3 2 1	020	27.60 (3.2)	-1.2	B	2513.24822	6 4 2 7 4 3	001	7.80 (3.9)	-0.6	5		
2292.78887	3	2 1 4 3 2	020	0.74 (4.0)	-3.9	5	2431.87136	6 1 5 5 2 4	020	9.85 (1.9)	1.9	8	2515.85504	9 5 5 8 4 4	020	2.13 (2.8)	1.9	3		
2296.87251	4	1 3 5 2 4	020	5.96 (0.5)	3.3	3	2431.93218	6 2 5 5 1 4	020	28.27 (3.0)	-2.7	9	2516.70377	7 6 2 6 5 1	020	7.49 (3.6)	-1.9	6		
2302.11549	4	1 4 5 0 5	020	33.33 (2.7)	0.9	3	2432.49213	B 2 6 8 1 7	020	3.17 (5.9)	6.0	4	2519.37190	9 5 4 8 6 3	020	2.75 (4.2)	5.9	4		
2311.80148	3	0 3 4 1 4	020	32.16 (2.5)	0.1	8	2432.50763	B 3 6 8 2 7	020	8.57 (3.9)	-4.4	6	2519.42683	4 2 5 4 1	001	7.47 (3.6)	-3.4	5		
2311.86703	3	1 3 4 0 4	020	11.38 (3.6)	5.8	B	2433.63445	5 2 3 4 3 2	020	17.94 (2.5)	-0.7	9	2520.50225	6 5 2 5 2 3	020	6.35 (2.9)	5.0	5		
2390.23645	3	3 1 3 2 2	020	6.62 (3.3)	7.0	5	2436.92519	9 4 5 9 3 6	020	4.49 (3.5)	-5.9	4	2520.52504	6 4 3 5 1 4	020	5.86 (1.5)	5.5	6		
2381.36767	3	1 2 3 0 3	020	17.19 (2.8)	-0.6	9	2437.02508	10 7 3 1 1 7 4	001	1.21 (4.3)	1.6	3	2522.57011	6 3 3 7 3 4	001	5.74 (1.0)	2.4	3		
2382.68870	5	4 1 5 3 2	020	22.86 (3.0)	-5.2	9	2430.78424	5 3 3 4 2 2	020	8.06 (1.7)	0.7	4	2522.87843	7 6 1 6 5 2	020	22.64 (3.0)	-4.7	6		
2383.11074	3	2 2 3 1 3	020	5.70 (4.7)	0.0	6	2441.25106	9 3 6 9 2 1	020	5.73 (5.0)	1.2	5	2525.73161	5 4 1 6 4 2	001	3.09 (1.5)	2.5	5		
2383.95549	4	2 2 4 1 3	020	7.41 (3.9)	-1.6	5	2441.32450	9 4 6 9 3 7	020	1.84 (4.0)	-2.8	3	2525.86174	7 5 2 6 4 3	020	11.04 (3.2)	-2.4	8		
2387.05167	5	3 2 5 2 3	020	20.53 (2.1)	-5.1	9	2441.67792	7 1 6 6 2 5	020	24.55 (3.3)	-1.1	8	2527.22756	10 5 6 9 4 5	020	4.11 (4.8)	0.4	5		
2387.68153	3	0 3 2 1 2	020	32.07 (3.6)	-1.8	5	2441.68817	7 2 6 6 1 5	020	8.32 (2.9)										

APPENDIX 11 (continued)

I	II	III	IV	V	VI	VII	I	II	III	IV	V	VI	VII	I	II	III	IV	V	VI	VII	
2578.29600	9	5	4	9	6	3	100	2.20	(3.5)	3.3	4	.	2650.11852	7	3	4	7	2	5	100	
2578.33872	1	1	0	2	2	1	100	5.99	(1.9)	0.5	3	.	2652.92764	3	1	2	2	2	1	100	
2578.36056	7	3	4	7	4	3	100	3.72	(5.2)	1.4	5	.	2652.95566	6	2	4	6	1	5	100	
2578.52668	2	2	0	3	2	1	001	4.51	(4.8)	-1.9	4	.	2653.13659	6	3	4	6	2	5	100	
2580.2149a	9	8	1	8	7	2	020	11.48	(1.7)	-3.1	8	.	2655.18044	5	1	4	5	0	5	100	
2580.44189	6	4	3	6	5	2	100	3.14	(4.9)	2.1	4	.	2655.30338	6	3	3	6	3	4	001	
2580.71018	2	1	2	3	0	3	100	9.56	(2.9)	-1.	5	8	2655.42558	4	0	4	3	1	3	100	
2581.17935	6	1	5	6	3	4	001	5.47	(5.2)	1.1	5	.	2655.47080	4	1	4	3	0	3	100	
2581.41044	6	2	5	6	2	4	001	1.73	(0.0)	-5.	1	2	2658.20958	3	2	2	2	1	1	100	
2582.54789	5	1	5	5	1	4	001	5.32	(0.2)	-4.1	2	.	2658.26890	11	6	5	1	0	5	020	
2502.83435	9	6	3	8	5	4	020	4.37	(0.1)	1.4	2	.	2658.32040	5	2	3	5	2	4	001	
2588. 85981	12	7	6	11	6	5	020	0.76	[3.5]	-2.	9	2	2658.45881	8	3	5	8	2	6	100	
2588.87158	7	4	3	7	5	2	100	7.05	(2.7)	1.5	4	.	2658.59094	8	4	5	8	3	6	100	
2589.56938	6	2	4	6	4	3	001	3.31	(4.4)	-2.	9	3	2661.40282	7	2	5	7	1	6	100	
2589.65984	1	0	1	2	1	2	100	9.33	(1.3)	1.3	3	.	2661.43582	7	3	5	7	2	6	100	
2589.72184	3	0	3	3	1	2	100	5.59	(4.0!)	6.0	4	.	2663.98396	4	1	3	3	2	2	100	
2589.89182	9	9	1	8	8	0	020	5.02	(0.4)	0.7	2	.	2665.56695	4	2	3	3	1	2	100	
2590.47281	5	2	3	5	3	2	100	9.26	(1.8)	-1.	2	6	2669.55128	3	3	1	2	2	0	100	
2591.14336	5	4	1	5	5	0	100	4.13	(4.3)	-1.3	5	.	2673.01558	8	3	5	8	3	6	001	
2597.00757	5	3	2	5	4	1	100	13.72	(1.6)	-2.3	5	.	2673.10576	5	1	4	4	2	3	100	
2599.31798	0	0	0	1	1	1	100	3.06	(0.1)	5.3	2	.	2673.42273	5	2	4	4	1	3	100	
2599.64091	4	2	2	4	3	1	100	5.88	(3.4)	0.0	5	.	2675.06305	3	3	0	2	2	1	100	
2600.65446	4	1	3	4	3	2	001	3.14	(3.2)	-4.5	3	.	2680.24446	5	2	3	4	3	2	100	
2606.44006	2	1	1	2	2	0	100	6.52	(2.4)	3.8	5	.	2681.57591	6	1	5	5	2	4	100	
2608.52128	10	10	0	1	0	1	001	0.72	(4.0)	-2.	5	3	2681.92503	3	2	1	2	1	2	100	
2609.58213	1	0	1	1	1	0	100	15.98	(2.5)	-1.	0	9	2688.94729	4	1	3	3	0	100		
2609.73257	10	9	2	9	8	1	020	6.56	(1.5)	-2.	0	3	2690.15789	6	2	4	5	3	3	100	
2619.75395	1	1	0	1	0	1	100	20.64	(3.6)	-0.6	9	.	2691.39564	6	3	4	5	2	3	100	
2620.44688	10	10	0	9	9	1	020	2.65	(2.7)	-1.	7	6	2693.28440	4	4	0	3	3	1	100	
2620.81892	2	2	0	2	1	1	100	8.31	(3.3)	0.8	5	.	2698.54609	5	4	2	4	3	1	100	
2622.85642	3	3	0	3	2	1	100	20.90	(2.1)	-0.4	9	.	2698.60808	7	2	5	6	3	4	100	
2624.08222	5	4	1	5	3	2	100	22.77	(3.7)	-2.	9	9	2698.87050	7	3	5	6	2	4	100	
2624.09617	4	3	1	4	2	2	100	9.96	(2.5)	2.	9	6	2699.25986	5	4	2	4	4	1	001	
2625.16642	3	2	1	3	1	2	100	26.36	(3.0)	-3.	7	9	2700.25341	12	6	7	11	3	8	020	
2625.43020	6	5	1	6	4	2	100	5.17	(2.9)	1.9	5	.	2702.31346	8	4	4	7	6	1	001	
2625.66329	7	5	2	7	4	3	100	13.84	[3.0]	-1.	9	8	2703.04402	12	5	8	1	2	9	020	
262 S. 79422	9	7	2	9	6	3	100	4.10	(4.2)	-2.	5	6	2703.42487	3	3	1	2	1	2	001	
2625.97672	4	4	0	4	3	1	100	4.96	(4.7)	0.6	4	.	2704.36012	5	4	1	4	4	0	001	
2626.79282	2	1	1	2	0	2	100	5.97	(3.4)	2.	2	5	2704.47240	7	2	6	6	2	5	001	
2627.75532	9	6	3	9	5	4	100	5.35	(4.0)	-3.	8	5	2704.47240	7	1	6	1	5	001		
2627' .91047	6	4	2	6	3	3	100	6.65	(1.7)	1.	7	5	2704.58785	6	4	3	5	3	2	100	
2628.12016	7	6	1	7	5	2	100	8.48	(2.9)	-0.2	5	.	2704.68995	13	12	1	1	2	1	1	020
2629.26838	1	1	1	0	0	0	100	6.17	(0.8)	4.	9	3	2705.59206	6	2	4	5	2	3	001	
2629.85984	5	5	0	5	4	1	100	9.76	(3.3)	2.1	6	.	2706.22961	7	3	4	6	4	3	100	
2630.42779	2	1	2	1	2	1	100	12.22	[2.9]	0.8	6	.	2706.56027	8	2	6	7	3	5	100	
2631.00168	5	3	2	5	2	3	100	22.08	(2.1)	-3.	1	9	2706.74289	7	4	3	6	5	2	100	
2632.37200	4	4	1	4	3	2	100	7.68	(0.6)	2.0	3	.	2709.73737	7	4	4	6	3	3	100	
2634.14877	4	2	2	4	1	3	100	7.61	(1.3)	3.0	5	.	2710.24639	5	5	1	4	4	0	100	
2635.63739	3	3	1	4	3	2	001	6.25	(3.1)	2.3	4	.	2713.132421	4	2	2	3	1	3	100	
2636.01753	10	6	4	1	0	5	5	100	0.98	(4.1!	-2.	2	3	2711.14177	6	4	3	5	4	2	001
2636.66496	3	1	2	3	0	3	100	15.67	(3.1)	-1.	9	6	2713.13406	7	3	5	6	3	4	001	
2636.77894	2	0	2	1	1	1	100	0.34	[1.7]	3.	5	5	2713.34564	7	2	5	6	2	4	001	
2636.80208	5	4	2	5	3	3	100	5.02	(5.4)	-0.2	4	.	2713.34564	9	5	4	8	7	1	001	
2637.29234	4	3	2	4	2	3	100	18.11	(3.4)	-2.	3	8	2713.55620	6	5	2	5	5	1	001	
2637.76543	6	6	1	6	5	2	100	6.21	(3.3)	1.	1	5	2713.85375	5	4	1	4	3	2	200	
2637.88454	3	2	2	3	1	3	100	5.10	(3.6)	1.	8	4	2714.47241	4	4	0	3	2	1	001	
2638.38823	2	1	2	1	0	1	100	28.94	(3.8)	-2.	4	9	2714.54829	4	3	1	3	1	2	001	
2640.85708	6	3	3	6	2	4	100	5.61	(5.0)	-1.	4	5	2715.07817	8	3	5	7	4	4	100	
2641.11709	6	4	2	6	4	3	001	6.73	(3.0)	2.	3	4	2716.00853	8	4	5	7	3	4	100	
2641.22471	10	8	3	1	0	7	4	100	2.03	(0.7)	8.	6	2	2716.71091	6	3	3	5	3	2	001
2643.99440	5	2	3	5	1	4	100	18.70	(2.1)	-1.	5	7	2717.30795	6	5	1	5	5	0	001	
2646.48035	3	0	3	2	1	2	100	46.88	(2.7)	-2.	4	7	2720.16923	13	2	12	23	1	13	100	
2646.79829	1	3	1	2	0	2	100	16.19	(2.4)	-0.	8	9	2720.16923	13	1	12	13	0	13	100	
2649.34996	2	2	1	1	0	0	100	33.49	(3.6)	-1.	7	8	2720.55629	12	0	12	11	1	11	100	

I	II	III	IV	V	VI	VII	I	II	III	IV	V	VI	VII	I	II	III	IV	V	VI	VII
2740.03393	6 4 2 5 3 3	100	5.96 (2.4)	-156.0	2	2757.48656	11 6 5 10 7 4	100	2.55 (2.5)	1.8	3	.	2785.79914	11 8 3 1 0 8 2	001	1.31 (2.9)	-2.2	3	.	
2740.03393	5 2 3 4 1 4	100	5.96 (2.4)	-156.0	2	2758.10947	6 4 3 5 1 4	100	7.45 (0.4)	1.0	2	.	2786.04761	11 8 4 1 0 7 3	100	2.10 (2.3)	2.8	2	.	
2740.15076	8 7 2 7 7 1	001	3.62 (2.1)	-0.6	3	2758.26611	9 7 2 8 7 1	001	3.79 (1.7)	2.2	2	.	2786.37758	8 6 2 7 4 3	001	1.25 (5.5)	-2.6	2	.	
2740.91494	7 6 2 6 5 1	100	5.67 (0.6)	3.4	3	2758.77893	5 5 0 4 2 3	100	0.75 (1.6)	2.0	2	.	2787.26806	10 8 3 9 7 2	100	4.84 (1.9)	2.9	3	.	
2740.97510	5 3 3 4 0 4	100	1.52 (2.0)	3.4	3	2759.51711	8 7 2 7 6 1	100	19.94 (3.2)	-3.1	6	.	2787.28377	7 7 1 6 5 2	001	1.76 (4.2)	-2.0	3	.	
2741.11737	5 3 2 4 1 3	001	1.73 (0.7)	3.2	3	2759.62958	9 5 4 8 5 3	001	0.73 (5.9)	-2.0	3	.	2788.75269	12 11 1 1 1 1 0	001	0.96 (1.8)	0.8	3	.	
2741.51167	8 7 1 7 7 0	001	10.69 (2.4)	-3.6	5	2760.41818	6 6 0 5 4 1	001	2.59 (1.6)	-0.7	2	.	2788.78117	7 5 3 6 3 4	001	2.25 (3.5)	-3.5	3	.	
2741.73181	8 4 4 7 4 3	001	3.84 (1.3)	0.2	3	2760.81508	10 6 5 9 6 4	001	1.19 (4.0)	2.3	3	.	2789.29573	12 8 5 1 3 7 4	100	2.68 (3.0)	4.8	3	.	
2742.40939	0 1 5 1 4 1 4	100	10.65 (1.9)	-2.0	5	2760.83070	11 5 7 10 5 6	001	1.17 (4.3)	0.3	3	.	2789.76609	12 10 2 1 1 0 1	001	1.44 (2.4)	-1.8	3	.	
2742.40939	1 5 1 5 1 4 0 1	100	10.65 (1.9)	-2.0	5	2760.86789	12 5 7 1 1 6 6	100	1.15 (4.4)	2.1	3	.	2792.16535	8 6 3 7 3 4	100	3.04 (0.8)	1.5	3	.	
2742.91761	2 13 13 1 1 12	100	9.84 (1.7)	-0.8	3	2761.44584	12 6 7 1 1 5 6	100	3.48 (2.3)	0.6	3	.	2792.70546	8 7 1 7 5 2	001	1.86 (2.2)	1.8	3	.	
2742.91761	1 6 1 3 1 3 2 1 2	100	9.84 (1.7)	-0.8	3	2761.48225	9 7 3 8 6 2	100	6.56 (0.9)	1.1	3	.	2793.40812	9 6 3 8 5 4	100	7.83 (1.2)	-0.2	3	.	
2743.60613	1 2 1 1 2 3 1 0	100	9.81 (3.0)	0.2	3	2761.91130	6 6 1 5 3 2	100	3.13 (0.7)	1.0	3	.	2794.68171	10 9 2 9 8 1	100	8.83 (1.6)	-2.0	3	.	
2743.60613	1 3 1 1 2 2 1 0	100	9.81 (3.0)	0.2	3	2762.51742	8 7 1 7 6 2	100	8.76 (0.7)	-0.3	3	.	2794.92473	10 8 2 9 7 3	100	2.70 (1.8)	1.0	3	.	
2744.28840	8 6 3 7 5 2	100	29.78 (2.9)	-4.5	6	2763.91637	16 3 14 15 2 13	100	1.69 (4.1)	0.8	3	.	2795.29442	12 9 3 1 1 9 2	001	1.88 (0.4)	4.6	3	.	
2744.47225	1 1 3 1 4 1 1 4	001	1.15 (1.2)	-3.1	2	2763.91637	16 2 14 15 3 13	100	1.69 (4.1)	0.8	3	.	2795.45908	10 9 1 9 8 2	100	3.18 (1.5)	1.0	3	.	
2744.47225	1 2 1 3 1 4 0 1 4	001	1.15 (1.2)	-3.1	2	2764.78773	8 8 1 7 7 0	100	30.57 (1.7)	-3.0	4	.	2795.80944	7 2 5 6 1 6	100	2.88 (1.3)	2.5	3	.	
2744.56592	12 3 9 1 1 4 8	100	10.07 (2.1)	-0.4	4	2764.90886	10 7 4 9 7 3	001	1.86 (3.2)	-6.6	3	.	2795.84412	7 3 5 6 0 6	100	0.95 (3.6)	1.8	2	.	
2744.56592	12 4 9 1 1 3 8	100	10.07 (2.1)	-0.4	4	2765.29602	10 9 1 9 9 0	001	4.03 (3.0)	-0.3	4	.	2798.30664	10 10 1 9 9 0	100	9.21 (1.3)	-4.3	3	.	
2744.71470	11 3 9 10 3 8	001	0.58 (3.6)	-5.6	2	2765.61487	10 8 3 9 8 2	001	2.03 (2.4)	0.2	3	.	2798.33529	10 10 0 9 9 1	100	3.09 (2.1)	-3.8	3	.	
2744.71470	11 2 9 1 0 2 8	001	0.58 (3.6)	-5.6	2	2765.92102	14 4 10 13 5 9	100	2.15 (3.2)	-1.2	3	.	2790.51058	1 3 4 6 1 5	001	0.88 (0.0)	-3.3	2	.	
2745.08545	0 5 5 9 6 4	100	2.40 (2.4)	2.6	3	2765.92102	14 5 10 13 4 9	100	2.15 (3.2)	-1.2	3	.	2798.62097	8 4 4 7 3 5	100	2.21 (2.6)	0.4	3	.	
2745.21011	5 5 1 4 3 2	001	2.51 (3.4)	-3.5	3	2766.31994	6 6 1 5 4 2	001	0.52 (2.7)	2.4	3	.	2798.90705	7 4 4 6 2 5	001	2.46 (0.9)	-0.4	3	.	
2745.27089	10 3 7 9 3 6	001	1.47 (4.8)	0.1	3	2766.90385	8 6 2 7 5 3	100	5.93 (0.8)	2.8	3	.	2798.93550	8 7 2 7 4 3	100	4.23 (1.7)	0.5	3	.	
2745.67572	9 5 5 8 5 4	001	4.09 (1.8)	0.3	4	2767.447.96	13 5 8 1 2 6 7	100	2.01 (3.3)	3.9	3	.	2799.28503	8 5 3 7 3 4	001	5.88 (1.2)	-0.3	3	.	
2745.84739	11 4 7 1 0 5 6	100	7.94 (4.0)	-1.9	5	2767.60515	13 6 8 12 5 7	100	0.68 (1.5)	4.4	2	.	2800.41688	12 8 4 1 1 8 3	001	2.44 (4.4)	-1.6	3	.	
2745.99171	7 6 1 6 5 2	100	34.44 (2. E)	-1.8	5	2767.64516	12 6 6 11 7 5	100	0.73 (2.2)	5.8	2	.	2800.48068	8 5 5 4 7 2	100	5.85 (2.2)	1.6	3	.	
2746.02650	11 5 7 1 0 4 6	100	2.68 (3.3)	-1.3	3	2768.20646	6 2 4 5 1 5	100	1.24 (1.9)	1.4	3	.	2804.30244	10 7 3 9 6 4	100	1.86 (2.5)	1.7	3	.	
2746.50322	5 4 2 4 2 3	001	2.33 (1.0)	0.9	3	2768.39557	6 3 4 5 0 5	100	3.74 (1.1)	3.0	3	.	2805.33085	11 9 3 1 0 8 2	100	1.14 (4.0)	0.5	3	.	
2746.95895	8 6 2 7 6 1	001	18.57 (2.21)	-4.7	6	2768.78694	9 6 3 8 6 2	001	0.78 (1.3)	-4.3	2	.	2805.61219	8 8 0 7 6 1	001	1.12 (2.4)	-1.0	3	.	
2747.17551	7 7 1 6 5 0	100	15.14 (2.3)	-1.	s 5	2768.80554	11 6 6 1 0 6 5	001	1.57 (0.7)	0.5	3	.	2809.70964	11 9 2 1 0 8 3	100	4.33 (1.8)	1.2	3	.	
2747.50342	7 7 0 6 6 1	100	45.99 (3.4)	-3.1	5	2769.88763	10 8 2 9 8 1	001	6.15 (1.4)	-0.3	3	.	2810.33509	7 3 5 6 1 6	001	1.46 (3.2)	5.8	3	.	
2747.57947	9 4 5 5 0 4 4	001	1.06 (2.4)	5.1	3	2769.27720	19 1 19 18 0 18	100	0.85 (4.3)	-2.2	2	.	2811.06069	11 10 2 10 9 1	100	1.44 (5.9)	-4.5	3	.	
2740.30669	9 6 4 8 5 3	100	5.41 (2.0)	-0.2	3	2769.27720	19 0 19 18 1 18	100	0.85 (4.3)	-2.2	2	.	2811.42988	11 10 1 10 9 2	100	4.48 (4.2)	-3.0	3	.	
2749.37231	16 0 16 15 1 15	100	6.29 (1.9)	0.7	3	2769.48170	7 4 3 6 3 4	100	10.41 (0.5)	-0.3	3	.	2811.53662	8 4 5 7 1 6	100	4.21 (1.6)	-1.1	3	.	
2749.37231	16 1 16 15 0 15	100	6.29 (1.8)	0.7	3	2769.75872	18 1 17 17 2 16	100	0.88 (0.6)	6.7	2	.	2811.69979	9 5 4 8 4 5	100	5.48 (0.6)	0.8	3	.	
2749.87287	15 2 14 14 1 13	100	5.79 (1.9)	0.6	3	2769.75672	18 2 17 17 1 16	100	0.88 (0.6)	6.7	2	.	2815.31254	11 8 3 1 0 7 4	100	3.28 (2.8)	-0.9	3	.	
2749.87287	15 1 14 1 4 2 1 3	100	5.79 (1.9)	0.6	3	2770.02709	11 7 5 1 0 6 4	100	1.67 (2.5)	1.2	3	.	2015.41624	9 6 3 8 4 4	001	1.79 (3.3)	2.6	3	.	
2750.24668	6 5 1 5 3 2	001	3.53 (0.7)	-0.6	3	2770.23256	6 3 3 5 1 4	001	3.57 (1.2)	0.1	3	.	2816.01817	9 6 4 8 3 5	100	1.33 (1.4)	1.1	3	.	
2750.53853	14 2 12 13 3 11	100	5.75 (1.6)	1.0	3	2770.35858	7 2 15 16 3 14	100	0.85 (3.5)	0.8	3	.	2016.06164	8 8 1 7 5 2	100	0.58 (4.5)	-5.4	3	.	
2750.53853	14 3 12 13 2 11	100	5.75 (1.6)	1.0	3	2770.35858	7 3 15 16 2 14	100	0.85 (3.5)	0.8	3	.	2825.96096	8 3 5 7 1 6	001	2.01 (0.5)	-0.7	3	.	
2751.28634	10 6 5 9 5 4	100	9.50 (0.13)	-0.2	3	2771.17124	16 3 13 15 4 12	100	0.95 (4.8)	2.6	2	.	2826.03420	0 4 5 7 2 6	001	0.64 (4.6)	-2.0	3	.	
2751.32127	9 6 4 8 6 3	001	7.94 (0.8)	-0.3	3	2771.17124	16 4 13 15 3 12	100	0.95 (4.8)	2.6	2	.	2826.15061	9 4 5 8 3 6	100	4.09 (1.2)	-0.2	3	.	
2751.45774	13 3 1 0 1 2 4 2 9	100	6.18 (1.5)	1.5	3	2771.98279	6 4 3 5 2 4	001	0.85 (0.6)	0.0	2	.	2826.62871	9 5 5 8 2 6	100	1.30 (3.0)	-0.8	3	.	
2751.45774	13 4 1 0 1 2 3 9	100	6.18 (1.5)	1.5	3	2772.54035	12 7 6 1 1 6 5	100	2.58 (3.5)	1.0	3	.	2826.70780	12 11 2 1 1 1 0 1	100	2.05 (2.3)	3.7	3	.	
2751.95984	6 5 2 5 2 3	100	2.58 (1.4)	4.6	3	2775.16444	7 5 3 6 2 4	100	2.28 (1.2)	1.7	3	.	2829.66010	12 12 1 1 1 1 0	100	2.40 (2.8)	0.9	3	.	
2752.15367	15 2 1 4 1 5 1 0 5 1	001	0.71 (2.8)	2.5	2	2775.19764	13 6 7 1 2 7 6	100	1.25 (1.2)	1.0	3	.	2829.66010	12 12 0 1 1 1 1	100	2.40 (2.8)	0.9	3	.	
2752.15367	15 1 1 4 1 5 1 1 5	001	0.71 (2.8)	2.5	2	2776.28751	7 6 2 6 3 3	100	2.93 (1.5)	-1.8	3	.	2829.88907	9 6 4 8 4 5	001	1.38 (2.2)	4.3	3	.	
2752.76170	12 5 8 1 1 4 7	100	5.09 (1.6)	0.9	3	2776.40009	12 5 7 1 1 5 6	001	0.70 (1.2)	1.2	3	.	2831.36703	10 7 4 9 4 5	100	1.71 (2.6)	-2.7	3	.	
2753.10979	9 7 3 8 7 2	001	9.97 (1.6)	-1.4	3	2777.07273	11 10 1 1 0 1 0 0	001	0.69 (2.9)	0.0	2	.	2832.65580	11 7 4 1 0 6 5	100	2.34 (3.0)	2.0	3	.	
2753.71234	11 5 6 1 0 6 5	100	5.46 (1.7)	2.1	3	2777.5														

APPENDIX 111 OBSERVED INTENSITIES OF THE 2ND TRIAD OF HYDROGEN SULFIDE

	11	111	IV	V	VI	VII	I	II	III	IV	V	VI	VII	I	II	III	IV	V	VI	VII
3383.75082	11	1 11 12 0 12	030	0.78 (3.9)	0.3 4 .	3539.45115	2 1 2 1 0 1	030	2.70 (2.5)	1.7 4 .	3623.07723	14 0 1 4 1 5 0 1 5	011	9.67 (3.0)	5.1 4 .					
3383.75062	11	0 11 12 1 12	030	0.78 (3.9)	8.3 4 .	3541.17617	4 3 1 4 2 2	030	0.88 (3.5)	0.2 4 .	3623.07723	14 1 1 4 1 5 1 1 5	011	9.67 (3.0)	5.1 4 .					
3406.59860	4	2 3 5 3 2	030	0.38 (5.4)	-1.3 4 .	3547.90962	3 0 3 2 1 2	030	3.68 (3.9)	1.4 4 .	3624.23332	10 8 2 11 8 3	011	3.93 (4.3)	4.0 5 .					
3407.85919	9	0 9 1 0 1 1 0	030	1.85 (3.8)	1.9 4 .	3551.20369	9 5 4 1 0 8 3	110	0.23 (2.4)	-3.4 3 .	3624.54422	6 3 3 5 4 2	030	0.15 (6.4)	7.4 2 .					
3407.65919	9	1 9 1 0 0 1 0	030	1.85 (3.8)	1.9 4 .	3555.28060	4 4 1 4 3 2	030	0.96 (5.5)	-4.6 4 .	3628.85664	7 7 0 8 8 1	110	17.19 (2.5)	-5.7 3 .					
3409.87480	7	7 1 8 8 0	030	0.22 (3.5)	2.9 2 .	3562.12484	9 5 5 10 7 4	011	0.65 (3.9)	2.6 3 .	3631.06152	12 1 1 1 3 2 1 2	110	8.66 (2.2)	-1.3 4 .					
3410.03374	7	7 0 8 8 1	030	0.62 (2.9)	-5.8 2 .	3563.03814	5 2 3 5 1 4	030	1.00 (3.2)	-2.7 4 .	3631.06152	12 2 11 13 1 12	110	8.66 (2.2)	-1.3 4 .					
3415.61073	6	6 1 7 7 0	030	1.20 (4.2)	-0.1 4 .	3575.20151	4 2 3 3 1 2	030	2.34 (3.2)	-0.2 5	3631.38788	10 6 4 1 1 6 5	011	1.99 (4.5)	5.3 4 .					
3416.26150	5	4 2 6 5 1	030	0.39 (4.2)	1.7 4 .	3577.09336	6 3 4 6 2 5	030	0.66 (5.4)	0.9 3 .	3632.26028	7 6 1 8 7 2	110	13.14 (3.9)	2.0 3 .					
3416.44270	9	1 8 1 0 2 9	030	1.04 (1.2)	2.7 4 .	3578.68406	7 4 3 7 3 4	030	0.49 (2.3)	-7.8 5 .	3634.51101	12 1 12 13 0 13	110	17.44 (2.4)	-3.3 5 .					
3416.44270	9	2 8 1 0 1 9	030	1.04 (1.2)	2.7 4 .	3578.71666	8 4 5 9 6 4	011	0.48 (1.5)	7.5 3 .	3634.51101	12 0 12 13 1 13	110	17.44 (2.4)	-3.3 5 .					
3419.41636	8	0 8 9 1 9	030	2.66 (3.5)	0.7 4 .	3578.74502	10 8 3 1 1 9 2	110	0.94 (5.7)	5.2 3 .	3636.31440	10 4 6 11 5 7	110	1.10 (5.1)	-3.7 5 .					
3419.41836	8	1 8 9 0 9	030	2.66 (3.5)	0.7 4 .	3582.21776	7 2 6 8 4 5	011	2.27 (5.3)	4.4 5 .	3636.38827	9 7 2 10 7 3	011	3.34 (4.6)	2.2 5 .					
3430.64087	7	0 7 8 1 8	030	3.47 (5.1)	-4.0 4 .	3582.21776	3 3 1 2 2 0	030	2.27 (5.3)	4.4 5 .	3638.75520	12 3 10 13 3 11	011	8.92 (2.9)	-2.1 5 .					
3430.64007	7	1 7 8 0 8	030	3.47 (5.1)	-4.0 4 .	3583.32294	16 1 16 17 0 17	110	1.34 (4.9)	3.6 4 .	3638.75520	12 2 10 13 2 11	011	8.92 (2.9)	-2.1 5 .					
3432.57035	4	4 1 5 5 0	030	2.64 (2.6)	0.4 4 .	3583.32294	16 0 16 17 1 17	110	1.34 (4.9)	3.6 4 .	3639.46343	10 5 5 1 1 5 6	011	6.43 (3.0)	2.7 5 .					
3436.36127	7	2 5 8 3 6	030	0.96 (4.1)	-6.5 2 .	3584.50069	7 2 5 8 5 4	110	1.09 (4.5)	-4.3 4 .	3644.37515	9 1 1 0 9 2	011	3.02 (4.3)	-2.2 5 .					
3436.46867	7	3 5 8 2 6	030	0.31 (5.9)	-8.6 2 .	3584.75560	6 6 1 6 5 2	030	0.31 (4.3)	6.3 3 .	3653.90239	10 3 7 1 1 3 8	011	19.82 (1.5)	5.4 3 .					
3437.97052	5	3 2 6 4 3	030	1.21 (1.8)	1.0 3 .	3584.99566	5 1 4 4 2 3	030	2.46 (0.4)	2.6 3 .	3653.90239	10 4 7 1 1 4 8	011	19.82 (1.5)	5.4 3 .					
3441.52217	6	0 6 7 1 7	030	4.47 (4.1)	-3.1 4 .	3585.36014	5 2 4 4 1 3	030	0.80 (4.0)	-1.2 4 .	3654.07934	10 1 9 1 1 2 1 0	110	25.40 (2.9)	-3.0 3 .					
3441.52217	6	1 6 7 0 7	030	4.47 (4.1)	-3.1 4 .	3589.69477	8 0 8 7 1 7	030	3.62 (5.4)	-1.1 5 .	3654.07934	10 2 9 11 1 10	110	25.40 (2.9)	-3.0 3 .					
3443.49871	6	1 5 7 2 6	030	0.68 (5.3)	-5.2 4 .	3589.69477	8 1 8 7 0 7	030	3.62 (5.4)	-1.1 5 .	3654.58783	11 2 10 12 2 11	011	28.75 (1.8)	-2.8 3 .					
3443.51732	6	2 5 7 1 6	030	2.13 (3.4)	-0.6 4 .	3594.06765	15 1 14 16 2 15	110	1.19 (5.3)	2.9 3 .	3654.58783	11 1 10 12 1 11	011	28.75 (la)	-2.8 3 .					
3448.10894	5	2 3 6 3 4	030	1.66 (3.2)	0.1 3 .	3594.86765	15 2 14 16 1 15	110	1.19 (5.3)	2.9 3 .	365 10475	8 7 2 9 7 3	011	5.31 (4.4)	3.8 3 .					
3451.81142	5	1 4 6 2 5	030	2.64 (1.5)	1.7 3 .	3594.95774	12 8 4 1 3 8 5	011	0.81 (4.1)	2.9 2 .	3659.05884	11 0 11 12 0 12	011	52.76 (2.7)	-3.0 4 .					
3452.05680	5	0 5 6 1 6	030	5.38 (5.6)	-1.7 4 .	3596.92441	9 0 9 8 1 8	030	2.66 (3.8)	-2.9 5 .	3659.05884	11 1 11 12 1 12	011	52.76 (2.7)	-3.0 4 .					
3452.05680	5	1 5 6 0 6	030	5.38 (5.6)	-1.7 4 .	3596.92441	9 1 9 8 0 8	030	2.66 (3.8)	-2.9 5 .	3659.54544	7 4 3 8 5 4	110	10.16 (0.4)	2.3 3 .					
3456.73729	2	2 1 3 3 0	030	2.63 (3.0)	5.3 3 .	3599.28824	5 2 3 4 3 2	030	1.08 (3.0)	0.3 3 .	3660.28423	8 6 3 9 6 4	011	8.10 (1.1)	4.1 3 .					
3459.58714	4	3 5 2 4 4	030	0.93 (4.8)	-1.9 4 .	3601.61163	15 4 12 16 4 13	011	0.55 (3.7)	7.9 2 .	3660.80441	5 4 2 6 5 1	110	2.74 (4.91)	-2.9 3 .					
3460.12050	2	2 3 5 1 4	030	2.83 (2.2)	0.5 4 .	3601.61163	15 3 12 16 3 13	011	0.58 (3.7)	7.9 2 .	3662.71960	8 3 5 9 4 6	110	5.74 (0.3)	8.5 3 .					
3466.33885	3	1 2 4 2 3	030	2.76 (3.0)	0.5 4 .	3601.97361	12 12 0 1 3 1 2 1	011	0.12 (1.6)	-4.3 2 .	3662.94974	8 4 5 9 3 6	110	17.14 (2.1)	4.6 3 .					
3468.66743	3	2 2 4 1 3	030	0.89 (2.5)	3.2 3 .	3603.79319	10 1 10 9 0 9	030	2.08 (2.5)	7.2 5 .	3663.61896	5 5 1 6 6 0	110	19.82 (2.8)	-2.2 6 .					
3469.73841	5	1 5 5 2 4	030	0.37 (5.2)	-0.7 3 .	3603.79319	10 0 10 9 1 9	030	2.08 (2.5)	7.2 5 .	3664.06730	4 2 3 5 3 2	110	7.44 (0.8)	2.3 3 .					
3469.78401	5	0 5 5 1 4	030	1.15 (1.6)	3.5 4 .	3604.38071	12 7 6 13 6 7	110	0.37 (5.0)	3.5 3 .	3664.33835	5 5 0 6 6 1	110	57.52 (3.2)	-3.1 5 .					
3472.02975	3	0 3 4 1 4	030	4.39 (3.8)	-1.0 4 .	3608.48463	15 2 14 16 2 15	011	1.98 (3.9)	-7.1 3 .	3664.56109	5 3 2 6 5 1	011	13.35 (2.1)	5.5 3 .					
3472.10753	1	1 3 4 0 4	030	1.50 (2.8)	1.7 4 .	3608.48463	15 1 14 16 1 15	011	1.98 (3.9)	-7.1 3 .	3664.58300	7 5 2 8 5 3	011	15.99 (1.6)	-0.1 3 .					
3472.18886	2	1 1 3 2 2	030	0.85 (4.2)	1.0 4 .	3609.82964	8 6 3 9 7 2	110	6.32 (3.2)	2.5 5 .	3664.64063	6 4 2 7 5 3	110	5.70 (1.4)	6.2 3 .					
3479.07306	2	2 1 3 2 2	030	1.51 (4.3)	2.1 4 .	3610.30527	11 1 11 10 0 10	030	1.22 (4.5)	-5.2 4 .	3665.06692	4 4 4 9 4 5	011	26.32 (3.0)	-0.6 5 .					
3479.84909	1	1 0 2 2 2	030	2.78 (3.3)	1.0 4 .	3610.30527	11 0 11 10 1 10	030	1.22 (4.5)	-5.2 4 .	3665.63962	10 2 9 11 2 10	011	49.12 (0.4)	-1.9 2 .					
3481.29355	2	0 2 3 1 3	030	1.33 (1.3)	4.4 4 .	3610.46199	11 7 4 12 7 5	011	0.74 (5.4)	-0.7 4 .	3665.37445	8 3 5 9 3 6	011	37.90 (3.9)	-3.5 5 .					
3489.11615	5	2 4 5 3 3	030	0.54 (2.8)	5.4 4 .	3611.05E047	12 6 7 13 5 8	110	0.56 (2.7)	2.6 3 .	3666.44503	7 6 1 8 6 2	011	11.34 (1.1)	2.9 3 .					
3490.07042	5	1 4 5 2 3	030	1.59 (5.5)	-0.5 3 .	3610.68948	15 1 15 16 1 16	011	4.63 (3.6)	1.0 5 .	3667.98136	7 5 3 8 4 4	110	9.57 (1.0)	5.0 3 .					
3491.85887	1	1 1 2 0 2	030	0.83 (2.4)	5.6 3 .	3610.68948	15 0 15 16 0 16	011	4.63 (3.6)	1.0 5 .	3672.33995	7 7 1 8 7 2	011	16.01 (2.1)	-3.6 5 .					
3493.77804	7	2 5 7 3 4	030	0.82 (5.0)	-2.4 5 .	3611.53467	6 2 5 7 4 4	011	0.99 (1.9)	6.0 3 .	3672.56570	7 6 2 8 6 3	011	32.16 (2.9)	-3.5 5 .					
3499.32981	6	3 4 6 4 3	030	1.21 (0.9)	1.5 3 .	3611.85627	4 4 1 3 3 0	030	1.87 (3.7)	-5.4 4 .	3672.85272	7 4 4 8 3 5	110	8.65 (0.2)	4.3 3 .					
3506.10074	4	3 2 4 4 1	030	1.42 (3.0)	4.5 4 .	3611.96676	8 8 1 9 9 0	110	8.48 (5.9)	0.8 5 .	3673.37445	8 3 5 9 3 6	011	37.90 (3.9)	-3.5 5 .					
3507.38897	3	1 2 3 2 1	030	3.31 (4.6)	0.2 4 .	3613.85617	6 2 4 5 3 3	030	0.39 (5.1)	0.3 3 .	3673.45525	8 4 5 9 4 6	011	13.36 (2.5)	0.6 5 .					
3508.64202	1	0 1 1 1 0	030	2.96 (2.3)	1.7 4 .	3615.35275	6 3 4 5 2 3	030	1.27 (5.8)	4.0 3 .	3676.49517	? 2 8 10 2 9	011	78.48 (0.3)	-2.1 3 .					</td

I	II	III	IV	V	VI	VII	I	II	III	IV	V	VI	VII	I	II	III	IV	V	VI	VII	
3683.15423	4 4 0 5 5 1	110	28.18 (3.7)	-3.3 5	3747.62668	9 6 4 9 7 3	110	2.97 (3.1)	4.2 2	3793.53027	5 5 0 5 5 1	011	105.60 (0.9)	-2.1 5 .							
3683.43715	6 4 3 7 3 4	110	37.49 (3.6)	-1.8 5 .	3747.79218	8 5 4 8 6 3	110	19.26 (2.5)	-3.4 5 .	3793.81424	1 1 0 1 1 1	011	82.54 (3.4)	2.8 3 .							
3683.99541	4 2 2 5 4 1	011	37.39 (3.3)	-4.6 3 .	3747.93576	7 3 5 7 3 4	011	39.96 (1.6)	-0.3 4	3794.03971	6 6 1 6 6 0	011	72.66 (1.9)	-0.9 5 .							
3685.72 972	5 3 2 6 4 3	110	29.91 (2.9)	-2.7 6	3748.58091	2 2 1 3 2 2	011	61.12 (3.0)	-2.2 6	3794 .32001	1 1 1 0 0 0	011	34.72 (2.2)	2.7 5 .							
3606.54144	6 6 1 7 6 2	011	11.12 (1.0)	0.1 3 .	3748.68953	6 2 4 6 3 3	110	18.31 (2.2)	0.6 5 .	3794 .62530	6 6 0 6 6 1	011	213.60 (1.2)	-3.5 5 .							
3686.85599	7 1 6 8 2 7	110	86.73 (1.1)	-1.1 3 .	3748.74611	8 5 3 8 7 2	011	2.22 (0.4)	-1.4 2 .	3795.11611	8 7 2 8 7 1	011	18.53 (2.9)	0.0 5 .							
3686.85599	7 2 6 8 1 7	110	86.73 (1.1)	-1.1 3 .	3154.72905	3 0 3 3 1 2	110	67.16 (1.4)	0.3 3 .	3795 .77420	7 7 1 7 7 0	011	124.20 (1.1)	-6.0 5							
3607.67516	6 5 2 7 5 3	011	20.98 (2.9)	-3.2 4	3755.88553	2 1 2 3 1 3	011	106.00 (1.4)	0.7 5 .	3795.97557	5 4 1 5 3 2	110	101.40 (1.5)	-0.3 5 .							
3689.72287	3 0 3 4 2 2	011	2.73 (4.2)	1.4 3 .	3756.06215	9 5 5 9 5 4	011	13.10 (0.4)	0.7 3	3796.04531	7 7 0 7 7 1	011	40.39 (2.9)	-9.0 6 .							
3689.96810	6 3 4 7 2 5	110	51.15 (1.7)	-3.0 4	3756.15078	5 2 4 5 2 3	011	79.10 (2.0)	1.6 5 .	3796.60999	4 4 0 4 3 1	110	23.00 (2.2)	0.7 2 .							
3692.65754	4 3 1 5 4 2	110	16.83 (3.1)	-1.9 5 .	3756.21113	6 5 2 6 6 1	110	42.57 (3.8)	-6.1 7	3796.73554	2 2 1 2 1 2	110	84.80 (1.9)	-3.6 5 .							
3692.75404	6 4 3 7 4 2	011	29.71 (2.4)	-1.5 5 .	3756.28016	6 2 4 6 4 3	011	54.24 (3.7)	-8.0 4	3797.28461	7 6 1 7 6 2	011	31.55 (3.0)	-4.5 7							
3693.44643	3 2 2 4 3 1	110	7.50 (1.1)	2.7 3 .	3756 .30389	1 1 1 2 0 2	110	36.67 (3.0)	-3.1 6 .	3798.50633	5 4 1 5 4 2	011	64.72 (3.3)	-1.7 5 .							
3694.18177	5 4 1 6 4 2	011	39.22 (0.8)	1.1 3 .	3757.17018	4 1 3 4 2 2	110	30.57 (2.2)	-1.0 5 .	3799.50609	3 3 1 3 2 2	110	63.20 (1.4)	1.6 5 .							
?697.747'04	5 5 0 6 5 1	011	20.02 (3.5)	-0.3 5	3757.76326	1 1 0 2 1 1	011	67.05 (3.0)	-0.2 5	3799.73204	4 3 1 4 3 2	011	240.60 (0.8)	-0.5 5 .							
3698.71958	5 2 3 6 3 4	110	56.67 (4.0)	-1.5 4 .	3760.75398	3 2 2 3 3 1	110	29.56 (1.8)	6.0 5 .	3802.53061	7 5 2 7 4 3	110	41.44 (3.7)	-3.0 7 .							
3699.09624	3 3 1 4 4 0	110	16.99 (0.4)	6.1 2 .	3761.18081	6 3 3 6 5 2	011	42.84 (1.3)	-1.4 4 .	3802.61818	4 2 2 4 1 3	110	31.48 (2.9)	-0.4 5 .							
3701.09877	5 5 1 6 5 2	011	57.19 (2.8)	-6. o 2	3761.93093	10 6 4 10 7 3	110	3.22 (5.8)	3.7 3	3802.66451	2 1 1 2 1 2	011	105.50 (1.3)	-0.4 5 .							
3702.77647	3 3 0 4 4 1	110	107.30 (1.8)	-2.4 5 .	3763.03657	5 4 1 5 5 0	110	74.35 (1.4)	-0.3 5 .	3804.42848	4 4 1 4 3 2	110	14.01 (3.0)	1.5 5 .							
3703.55317	5 4 2 6 4 3	011	109.80 (2.7)	-3.2 5 .	3763.11212	7 5 2 7 6 1	110	49.54 (2.2)	-1.9 6 .	3804.58656	8 6 2 8 6 3	011	41.96 (3.4)	1.0 4 .							
3706.36628	4 2 2 5 3 3	110	19.22 (3.2)	-0.7 3 .	3763.20195	5 2 3 5 4 2	011	23.52 (3.7)	1.2 6	3804.62944	3 2 2 3 1 3	110	28.27 (4.0)	3.3 6							
3707.45962	5 1 4 6 2 5	110	101.40 (2.1)	-2.7 5 .	3763.04458	4 1 3 4 3 2	011	90.52 (1.2)	-0.9 5	3805.56833	8 6 2 8 5 3	110	7.74 (1.4)	7.4 3 .							
3707.51748	5 2 4 6 1 5	110	34.58 (3.2)	-1.2 7 .	3764.07616	0 0 0 1 1 1	110	30.17 (3.8)	-4.2 5	3806.25526	4 3 2 4 2 3	110	110.50 (2.1)	-1.6 5 .							
3707.84748	6 1 S 7 1 6	011	229.40 (0.8)	0.8 5 .	3764.51260	7 4 3 7 5 2	110	61.35 (0.5)	-1.4 3 .	3806.62249	7 5 2 7 5 3	011	23.16 (3.1)	-3.2 6							
3707.84748	6 2 5 7 2 6	011	229.40 (0.8)	0.8 5 .	3765.01458	1 0 1 2 0 2	011	85.88 (3.0)	8.4 3	3808.29943	5 4 2 5 3 3	110	46.51 (1.4)	1.3 3 .							
3709.83641	2 1 2 3 2 1	110	13.14 (1.8)	-0.7 3 .	3766.96128	4 3 1 4 4 0	110	37.44 (3.2)	-2.6 5 .	3808.49074	6 4 2 6 4 3	011	119.70 (2.0)	-1.6 5 .							
3711.22513	4 0 4 5 4 1	011	99.89 (2.4)	-0.6 5 .	3767.26788	3 1 2 3 2 1	110	161.90 (0.1)	5.5 3	3809.35940	5 5 1 5 4 2	110	6.43 (1.0)	6.3 3							
3711.33026	4 3 2 5 2 3	110	78.49 (2.4)	-1.1 5 .	3767.69966	4 2 3 4 2 2	011	36.96 (3.1)	-1.0 5 .	3810.78251	9 6 3 9 5 4	110	11.17 (3.7)	-0.3 2							
3713.59185	3 2 1 4 3 2	110	70.17 (1.1)	-0.5 3 .	3767 .00795	5 3 2 5 4 1	110	138.60 (0.3)	0.1 3 .	3810.89169	3 3 1 3 1 2	011	73.40 (3.8)	-0.8 5 .							
3715.76432	9 3 7 9 4 6	110	3.88 (3.3)	8.2 3 .	3769.14636	8 5 4 8 5 3	011	9.13 (1.2)	4.7 3 .	3811.48766	3 0 3 2 1 2	110	23.00 (0.7)	0.3 5 .							
3715.80216	9 2 7 9 3 6	110	10.51 (1.4)	-1.8 3 .	3769.21868	11 7 5 11 7 4	011	2.79 (2.1)	8.3 2	3811.81354	3 1 3 2 0 2	110	71.81 (0.4)	1.3 5 .							
3717.24121	4 1 3 5 2 4	110	36.79 (3.0)	-1.9 7 .	3769.60428	3 1 2 3 3 1	011	22.67 (2.3)	1.8 6	3812.26057	2 1 2 1 1 1	011	76.48 (0.9)	1.0 5 .							
3717.58872	4 2 3 5 1 4	110	115.90 (0.9)	-0.6 5 .	3770.16716	3 2 1 3 3 0	110	189.60 (0.9)	0.0 3	3812.38962	7 4 3 7 3 4	110	34.84 (2.5)	-2.2 6							
3717.64121	2 2 1 3 3 0	110	78.28 (1.3)	0.3 5 .	3771.42398	5 3 3 5 3 2	011	104.90 (1.6)	-0.8 5	3812.91458	4 2 2 4 2 3	011	89.37 (0.5)	-1.3 4 .							
3717.86553	5 1 4 6 1 5	011	70.63 (2.3)	1.0 5 .	3771.93632	2 0 2 2 2 1	011	72.21 (1.6)	0.8 5 .	3813.47998	3 1 2 3 1 3	011	28.40 (2.4)	-1.7 3 .							
3717.89167	5 2 4 6 2 5	011	210.00 (1.01)	-0.3 5 .	3772.30860	2 1 1 2 2 0	110	59.97 (3.6)	0.2 5	3813.62826	4 2 3 4 1 4	110	66.83 (2.0)	-1.7 5 .							
3717.98925	4 2 2 5 2 3	011	161.40 (2.2)	1.2 5 .	3773.48203	1 0 1 1 0 0	110	145.20 (0.1)	0.7 3 .	3813.64876	5 2 3 5 1 4	110	74.47 (2.4)	1.7 5 .							
3719.73006	2 0 2 3 2 1	011	20.64 (3.6)	1.3 4 .	3775.49113	9 6 4 9 6 3	011	14.00 (1.8)	0.9 3 .	3816.50363	4 3 2 4 1 3	011	34.40 (1.4)	-3.4 3 .							
3720.25149	4 3 2 5 3 3	011	57.24 (3.3)	-2.4 4 .	3775.52285	0 0 0 1 0 1	011	163.80 (1.0)	1.5 5 .	3816.96099	4 4 1 4 2 2	011	14.28 (2.9)	-1.4 5 .							
3723.07670	2 2 0 3 3 1	110	38.33 (2.8)	-3.0 3 .	3775.99194	6 4 3 6 4 2	011	26.97 (3.9)	-2.6 6 .	3817.49713	7 6 2 7 5 3	110	3.01 (1.2)	8.7 3 .							
3723.57026	2 1 3 3 0 0	011	50.50 (2.9)	-2.0 5 .	3776.21053	2 1 2 2 1 1	011	40.60 (3.7)	-1.2 5 .	3817.87781	7 5 3 1 4 4	110	19.46 (3.0)	0.3 5 .							
3727.59454	4 1 3 5 1 4	011	236.90 (0.2)	0.7 3 .	3778.78606	3 2 2 3 2 1	011	187.30 (0.0)	1.3 3 .	3819.47488	3 1 2 2 2 1	110	89.65 (2.9)	-0.8 5 .							
3127.77123	4 2 3 5 2 4	011	74.78 (2.1)	-6.8 3 .	3781.10412	7 5 3 1 5 2	011	55.77 (2.4)	-1.9 4 .	3819.57619	5 4 2 5 2 3	011	80.62 (1.5)	0.0 5 .							
3727.93102	3 2 1 4 2 2	011	43.50 (1.4)	0.0 2 .	3785.58191	5 4 2 5 4 1	011	175.40 (1.0)	-0.6 5 .	3820.27473	4 0 4 3 1 3	110	88.10 (3.7)	1.9 5 .							
3727.95433	3 2 2 4 1 3	110	38.97 (2.0)	1.6 2 .	3786.35785	8 6 3 8 6 2	011	11.96 (1.3)	1.3 3 .	3820.32139	4 1 4 3 0 3	110	257.60 (0.5)	-0.5 5 .							
3737.28082	8 3 6 8 3 5	011	8.32 (2.7)	2.7 3 .	3786.61254	2 2 1 2 2 0	011	116.60 (2.6)	-0.2 5 .	3821.58685	2 L 1 1 1 0	011	267.30 (0.2)	1.8 5 .							
3737.34544	7 2 5 7 3 4	110	30.97 (2.8)	-5.9 2 .	3787.27722	2 2 0 2 1 1	110	S3.47 (2.5)	-1.6 6 .	3822.04257	3 0 3 2 0 2	011	124.30 (2.2)	0.8 5 .							
3737.73589	3 2 2 4 2 3	011	246.70 (0.2)	0.7 3 .	3788.55613	3 3 1 3 3 0	011	414.00 (0.3)	0.3 5 .	3822.73838	5 1 4 5 0 5	110	55.81 (1.2)	3.3 4 .							
3738.71428	A 4 5 8 5 4	110	19.86 (2.1)	-4.9 5 .	3789.15650	6 5 2 6 5 1	011	44.97 (1.3													

APPENDIX 111 (cont inued)

1	11	111	Iv	V	VI	VII	I	11	111	Iv	v	VI	VII	1	11	111	IV	v	VI	VII					
3830.67653	4	1	4	3	1	3	011	147.60	(2.0)	1.9	5	.	3867.37110	4	3	1	3	2	2	110	21.32	(2.7)	-0.7	4	.
3830.71350	4	0	4	3	0	3	011	438.30	(0.7)	0.7	5	3876.81375	8	2	7	7	2	6	011	271.70	(0.6)	1.3	2	.	
3830.99251	3	2	2	2	2	1	011	1B6.10	(0.6)	1.3	5	.	3876.81375	8	1	7	7	1	6	011	271.70	(0.6)	1.3	2	.
3831.11332	4	1	3	3	2	2	110	52.29	(2.0)	0.2	6	.	3877.57850	6	4	3	5	3	2	110	52.82	(2.7)	-0.2	6	.
3832.74977	4	2	3	3	1	2	110	157.70	(0.7)	0.8	5	3878.47333	10	1	10	9	1	9	011	228.10	(1.3)	-0.6	5	.	
3832.87329	7	2	5	7	1	6	110	39.49	(3.3)	-0.7	7	,	3878.47333	10	0	1	0	9	0	011	228.10	(1.3)	-0.6	5	.
3832.91800	7	3	5	7	2	6	110	13.72	(2.3)	2.8	4	3878.64307	4	3	1	3	1	2	011	78.13	(0.8)	1.9	5	3924.84005	
3832.98697	8	6	3	8	4	4	011	7.87	(2.3)	7.0	3	.	3878.70780	8	2	6	7	3	5	110	27.24	(2.6)	2.8	5	3928.34469
3833.11588	5	1	4	5	1	5	011	20.18	(3.2)	0.3	6	3878.76100	8	3	6	7	2	5	110	79.45	(1.2)	0.2	5	? 928.78559	
3833.15057	5	2	4	5	0	5	011	58.79	(3.1)	-3.3	6	3879.29367	4	2	2	3	1	3	110	5.02	(1.9)	5.2	3	3929.14558	
3833.80444	3	1	2	2	1	1	011	103.60	(1.1)	0.4	5	3880.66868	7	3	5	6	3	4	011	177.20	(1.0)	0.7	5	3930.31676	
3S33.96004	8	3	5	8	2	6	110	9.08	(0.8)	4.1	3	3880.86834	7	2	5	6	2	4	011	63.03	(1.6)	5.8	4	3930.39952	
3s34. 04430	6	2	4	6	2	5	011	59.90	(2.6)	-2.4	5	.	3882.38440	7	4	3	6	5	2	110	29.38	(2.3)	-0.7	5	3933.86378
3834.14123	8	4	5	8	3	6	110	25.74	(3.0)	-3.9	6	3883.66307	5	5	1	4	4	0	110	79.40	(1.5)	-1.7	5	3936.65175	
3836.78964	6	0	6	5	1	5	110	353.30	(0.6)	0.7	5	3804.03441	7	4	4	6	3	3	110	19.18	(2.7)	-0.3	3	3937.65498	
3836.78964	6	1	6	5	0	5	110	353.30	(0.6!)	0.7	5	3884.07077	8	6	2	7	7	1	110	1.00	(7.0)	-3.7	2	3939.77997	
3837.52966	3	3	1	2	2	0	110	14.33	(0.3)	5.0	2	3885.25283	5	5	0	4	4	1	110	217.20	(1.9)	-0.7	5	3941.15798	
3840.38095	7	1	6	7	0	7	110	39.47	(1.3)	-2.6	3	3885.32711	6	3	3	5	3	2	011	210.30	(1.6)	-0.1	5	3943.47603	
3840.38095	7	2	6	7	1	7	110	39.47	(1.3)	-2.6	3	3888.77158	6	5	1	5	5	0	011	46.03	(1.1)	-0.5	6	3945.40406	
3840.64352	5	1	4	4	2	3	110	178.00	(1.0)	0.3	5	3889.49502	0	2	6	7	2	5	011	135.70	(2.1)	-0.7	5	3945.73961	
3841.64297	4	2	3	3	2	2	011	104.90	(2.7)	8.4	4	.	3889.90878	4	2	2	3	0	3	011	13.95	(1.6)	4.9	3	3946.19847
3842.75566	4	1	3	3	1	2	011	319.00	(1.0)	0.9	5	3890.51929	6	4	2	5	4	1	011	44.75	(1.2)	1.2	6	3947.60813	
3843.27637	3	3	0	2	2	1	110	122.30	(1.3)	-1.7	5	3090.58009	8	3	5	7	4	4	110	17.57	(2.4)	1.0	5	3948.90050	
3845.94929	9	5	5	9	3	6	011	17.42	(3.5)	8.6	2	3890.90442	4	4	1	3	2	2	011	9.45	(0.7)	4.8	3	3949.30321	
3847.30556	4	3	2	3	2	1	110	93.34	(0.4)	6.0	4	3891.55892	8	4	5	7	3	4	110	48.08	(2.4)	-5.1	3	3958.95494	
3847.55670	6	1	6	5	1	5	011	574.40	(0.5)	0.2	5	3892.51682	12	1	12	11	1	11	011	100.40	(1.4)	-1.7	5	3959.65898	
3847.55670	6	0	6	5	0	5	011	574.40	(0.5)	0.2	5	3892.51682	12	0	12	11	0	11	011	100.40	(1.4)	-1.7	5	3963.81114	
3848.77608	8	1	7	8	0	8	110	27.22	(0.4)	-3.9	3	3893.17906	4	3	2	3	1	3	011	5.78	(0.4)	7.3	3	3964.91973	
3848.77608	8	2	7	8	1	8	110	27.22	(0.4)	-3.9	3	3895.00112	10	2	8	9	3	7	110	54.47	(1.2)	1.5	3	3965.52750	
3851.07565	5	2	4	4	2	3	011	317.80	(0.6)	1.1	5	3895.00112	10	3	8	9	2	7	110	54.47	(1.2)	1.5	3	3965.74611	
3851.12923	7	1	6	7	1	7	011	42.86	(1.7)	-1.4	5	3895.44943	6	5	2	5	4	1	110	213.10	(1.8)	-0.7	5	3967.21024	
3851.12923	7	2	6	7	0	7	011	42.86	(1.7)	-1.4	5	3896.72775	5	3	2	4	2	3	110	26.24	(2.2)	-1.0	2	3968.70963	
3851.31938	5	1	4	4	1	3	011	107.40	(2.1)	1.1	5	3896.61523	8	4	4	7	5	3	110	11.43	(0.6)	3.9	3	3969.28237	
3855.63813	7	1	7	6	1	6	011	503.70	(0.6)	0.1	5	3898.97572	7	5	3	6	5	2	011	60.80	(0.1)	2.1	3	3972.45978	
3855.63813	7	0	7	6	0	6	011	503.70	(0.6)	0.1	5	3899.80530	9	4	6	8	3	5	110	13.01	(1.5)	2.7	3	3973.31708	
3856.30737	4	3	1	3	3	0	011	80.23	(1.6)	0.4	5	3900.37980	11	2	10	10	2	9	011	90.32	(3.0)	-1.6	5	3973.38853	
3859.49883	9	0	9	8	1	8	110	196.40	(1.5)	0.1	5	3900.37980	21	1	10	0	1	9	011	90.32	(3.0)	-1.6	5	3976.86602	
3059.49883	9	1	9	8	0	8	110	196.40	(1.5)	0.1	5	3901.31597	8	4	5	7	4	4	011	31.16	(2.6)	-1.2	5	3978.77441	
3859.75814	8	1	7	8	1	8	011	28.13	(3.0)	-5.1	3	3902.44931	7	6	2	6	6	1	011	22.24	(3.2)	-6.2	2	3986.89594	
3859.75814	8	2	7	8	0	8	011	26.13	(3.0)	-5.1	3	3902.74085	11	2	9	1	0	3	011	34.20	(2.6)	-0.8	4	3987.08697	
3859.93856	6	2	5	5	2	4	011	98.73	(3.3)	0.2	5	3902.74085	11	3	9	10	2	8	110	34.20	(2.6)	-0.8	4	3987.45064	
3859.98106	6	1	5	5	1	4	011	297.50	(2.6)	0.4	5	3904.81613	6	5	1	5	4	2	110	33.47	(3.9)	-2.0	6	3988.10234	
3860.81208	6	2	4	5	3	3	110	36.55	(2.7)	-1.5	7	3906.22965	10	3	8	9	3	7	011	87.87	(2.7)	-0.3	4	3997.51163	
3861.00382	4	4	1	3	3	0	110	314.30	(0.9)	-0.1	5	3906.22965	10	2	8	9	2	7	011	87.87	(2.7)	-0.3	4	4005.97380	
3861.19561	5	3	3	4	3	2	011	200.00	(1.0)	0.6	5	3906.29300	6	6	1	5	5	0	110	182.30	(0.7)	0.5	4	4006.60729	
3861.24375	9	2	7	9	2	8	011	22.63	(1.3)	-5.3	3	3906.44098	7	4	3	6	4	2	011	55.94	(3.9)	1.5	6	4008.89467	
3861.24375	9	3	7	9	1	8	011	22.63	(1.3)	-5.3	3	3907.07193	6	6	0	5	5	1	110	57.79	(1.5)	-1.0	5	4014.96648	
3862.10206	6	3	4	5	2	3	110	108.60	(1.2)	0.5	5	3908.30774	5	3	2	4	1	3	011	4.37	(4.5)	7.9	4	4015.12119	
3863.48511	8	1	8	7	1	7	011	407.10	[1.6]	-1.2	5	3909.68872	5	2	3	4	1	4	110	10.09	(2.9)	1.8	4	4016.74185	
3863.48511	8	0	8	7	0	7	011	407.10	(1.6)	-1.2	5	3910.36358	9	4	6	8	4	5	011	67.23	(1.2)	0.5	3	4017.08015	
3863.97264	5	2	3	4	2	2	011	86.64	(2.6)	-0.6	5	3910.52452	9	3	6	8	3	5	011	22.91	(3.8)	1.7	6	4017.14289	
3865.83167	8	1	7	7	2	6	110	165.10	(1.0)	1.6	3	3910.546B3	9	4	5	8	5	4	110	25.56	(3.9)	0.8	6	4024.15245	
3865.83167	8	2	7	7	1	6	110	165.10	[1.0]																